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ABSTRACT

A new technique is proposed for the generation of the isotropic and linearly anisotropic components of transfer matrices for elastic and discrete inelastic scattering. It enables some angular integrals to be expressed in terms of functions which can be calculated by the use of recurrence relations or series expansions instead of numerical quadratures.

1. INTRODUCTION

Efficient generation of transfer matrices for use in reactor calculations has been the subject of extensive studies for the last twenty years. A review of the techniques used for generating transfer matrices in computational codes has recently been completed [1]. In general, since the mechanisms of elastic and discrete inelastic scattering are most important in the generation of transfer matrices, efforts were concentrated on the search for new techniques which could be used to treat these mechanisms with accuracy without irreparably sacrificing computational efficiency. Thus, for example, the treatment of discrete inelastic scattering evolved from the simplified model [2] adopted in the MC^2 code, where scattering is considered to be isotropic in the laboratory system, for the fixed-angle model [3] used in the MC^2-2 code. The majority of the existing computational codes use different techniques for treating elastic and discrete inelastic scattering. This is due basically to the fact that certain possible simplifications in the treatment of elastic scattering do not apply to the case of discrete inelastic scattering. Mention may be made, among others, of the simplifications resulting from the use of a group structure with constant lethargy width which were tried out by the MC^2 and MC^2-2 codes or of difficulties inherent in discrete inelastic scattering, like the double-energy region [4]. An exception to this rule is the unified treatment [5] provided by the NJOY system where representation in the centre-of-mass system avoids the difficulties caused by the double-energy region in the treatment of discrete inelastic scattering. The flexibility afforded by the NJOY in the choice of the group structure is more advantageous than the use of a separate treatment for elastic scattering as in the MC^2.

In this study a new technique is proposed for generating the isotropic and linearly anisotropic components of transfer matrices for elastic and discrete inelastic scattering. The formulation used is similar to the unified treatment provided by the NJOY except that the angular integrals are expressed in terms of functions which can be calculated by recurrence relations or series expansions, as opposed to calculation by numerical integration as in the NJOY. It is hoped that the treatment developed here will, after it is implemented, be useful in the generation of transfer matrices suitable for fast reactors.

2. ANALYSIS

The collision cross-section for transfer of neutrons from group g' with energy $E'\epsilon(E_{g'},E_{g'-1})$ to group g with energy $E\epsilon(E_g,E_{g-1})$ through elastic or discrete inelastic scattering is given by

$$\sigma_x(g'\to g,\mu) = [2\pi\, W_{g'}]^{-1} \int_{E_{g'}}^{E_{g'-1}} dE'\; W(E')\; \sigma_x(E') \int_{E_g}^{E_{g-1}} dE\; f_x(E'\to E,\mu) \tag{1}$$

where $\sigma_x(E')$ is the collision cross-section for mechanism x at energy E', $f_x(E'\to E,\mu)$ describes the probability of a neutron of energy E' giving rise by mechanism x to a neutron of energy E, the angle between the directions of the initial and the final motion in the laboratory system is given by $\cos^{-1}\mu$ and W(E') is the weighting function, with $W_{g'}$ given by the integral of W(E') over group g'. If x = m, the mechanism considered is that of elastic scattering, while x = n'i denotes discrete inelastic scattering involving the excitation level i of the scattering nucleus. Distribution $f_x(E' \to E,\mu)$ is normalized so that the integral over all possible final energies and over $\mu \epsilon [-1,1]$ yields unity. Considering the known relationship [4] between μ and ω, the cosine of the scattering angle in the centre-of-mass system

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

with

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

where A is the ratio between the mass of the scattering nucleus and that of the neutron and $Q_i \leqq 0$, i = 0, 1, ... I, is the energy of excitation of level i of the scattering nucleus (i = 0 is a fictitious level with $Q_o = 0$, representing elastic scattering), we can formally write

$$f_x(E' \to E,\mu) = f_x(E' \to E)\quad \delta\ [\ \mu - S(\omega,E')\ ] \tag{4}$$

where

$$S(\omega,E') = \frac{1 + \gamma(E')\omega}{[\ 1 + 2\gamma(E')\omega + \gamma^2(E')\ ]^{1/2}} \quad . \tag{5}$$

Using the transformation

$$f_x(E' \to E) = f_x(E',\omega)\ \left|\ \frac{d\omega}{dE}\ \right| \tag{6}$$

and representing $f_x(E',\omega)$ by an expansion in Legendre polynomials truncated after (L + 1) terms, Eq. (4) can be written as

$$f_x(E' \to E,\mu) = \frac{1}{2}\ \delta[\mu - S(\omega,E')\ ]\ \frac{d\omega}{dE}\ \sum_{\ell=0}^{L}\ (2\ell+1)\ f_x(E',\ell)\ P_\ell(\omega) \quad , \tag{7}$$

where $f_x(E',\ell)$ are the coefficients of expansion of $f_x(E',\omega)$. It is to be noted that the absolute value used in Eq. (6) was removed from Eq. (7) because from the relation [4]

$$E = \frac{E'}{(A+1)^2} \left[1 + 2\gamma(E')\omega + \gamma^2(E') \right] \tag{8}$$

it is easy to verify that, for fixed E', E increases monotonically with ω. Figure 1 shows the variation of final energy E with initial energy E' for various values of $\omega\epsilon[-1,1]$ in the case of inelastic scattering involving the first level of $^7Li(Q_1 = -0.478$ MeV). The threshold energy for inelastic scattering $E_\ell = -(A+1)Q_i/A$, in this example, is approximately equal to 0.546 MeV. The threshold energy of backscattering $E_r = -A\,Q_i/(A-1)$*/ corresponds to point B in the graph. In the case of elastic scattering points A and B coincide and move towards the origin of the (E',E) plane and the family of curves represented in the graph degenerates into a family of straight-line segments.

Using the expression for $f_x(E'\to E,\mu)$ given by Eq. (7) in Eq. (1) and considering the sub-interval of integration over E' for which the integrand does not vanish, we obtain

$$\sigma_x(g'\to g,\mu) = [4\pi W_{g'}]^{-1} \int_{E^*_{g'}}^{E^*_{g'-1}} dE'\; W(E')\; \sigma_x(E') \sum_{\ell=0}^{L} (2\ell+1)\; f_x(E',\ell)$$

$$\times \int_{\omega(E_g,E')}^{\omega(E_{g-1},E')} d\omega\; P_\ell(\omega)\;\; \delta[\,\mu - S(\omega,E')\,] \quad , \tag{9}$$

where $E^*_{g'} = \max(E_{g'},E_\ell)$, $E^*_{g'-1} = \max(E_{g'-1},E_\ell)$ and the limits of integration over ω are determined with the help of Eq. (8). In practice,

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*/ Translator's note: The subscript r presumably stands for "retroespalhamento" meaning "backscattering".

instead of the direct use of $\sigma_x(g' \to g, \mu)$, it is customary to expand $\sigma_x(g' \to g, \mu)$ in Legendre polynomials and to utilize the components of the expansion

$$\sigma_x(g' \to g, k) = 2\pi \int_{-1}^{1} d\mu \, P_k(\mu) \, \sigma_x(g' \to g, \mu), \quad k = 0,1,\ldots,K. \tag{10}$$

Substitution of Eq. (9) into Eq. (10) results in

$$\sigma_x(g' \to g, k) = W_{g'}^{-1} \int_{E^*_{g'}}^{E^*_{g'-1}} dE' \, W(E') \, \sigma_x(E') \, F_k(E', g) \tag{11}$$

where

$$F_k(E', g) = \frac{1}{2} \sum_{\ell=0}^{L} (2\ell+1) \, f_x(E', \ell) \, X_{k,\ell}(E', g) \quad . \tag{12}$$

In Eq. (12), functions $X_{k,\ell}(E',g)$ are defined as

$$X_{k,\ell}(E', g) = \int_{\omega_g(E')}^{\omega_{g-1}(E')} d\omega \, P_k \left[S(\omega, E') \right] \, P_\ell(\omega) \quad , \tag{13}$$

where $\omega_g(E') = \max \{ -1, \min[\omega(E_g, E'), 1] \}$ and $\omega_{g-1}(E') = \min \{1, \max[\omega(E_{g-1}, E'), -1] \}$. Extensive studies [6, 7] were made of the special case of Eq. (13) where $\omega_g(E') = -1$ and $\omega_{g-1}(E') = 1$. In practice, only the isotropic ($k = 0$) and linearly anisotropic ($k = 1$) components of $\sigma_x(g' \to g, \mu)$ are important for reactor calculations. For this reason, the present work is confined to the study of these components. The problem reduces to calculating functions $X_{o,\ell}(E',g)$ and $X_{1,\ell}(E',g)$ since $\sigma_x(E')$ and $f_x(E',\ell)$ are supplied or calculated from basic data stored in libraries like ENDF/B [8] and the weighting function $W(E')$ is chosen from among simple forms such as $E^n, n = -1, 0, 1$ or pre-calculated and supplied in tabular form. For k = 0, it is possible to show with the help of the properties of the Legendre polynomials [9] that the functions

$$X_{0,\ell}(E',g) = \int_{\omega_g(E')}^{\omega_{g-1}(E')} d\omega \; P_\ell(\omega) \tag{14}$$

are given by

$$X_{0,\ell}(E',g) = \left(\frac{1}{2\ell+1}\right) \left[P_{\ell+1}(\omega) - P_{\ell-1}(\omega) \right] \Bigg|_{\omega_g(E')}^{\omega_{g-1}(E')} \tag{15}$$

with $P_{-1}(\omega) = 0$. Equation (15) can be used to calculate the functions $X_{o,\ell}(E',g)$ required in Eq. (12) with k = 0. For k = 1 it is advantageous to define

$$Y_\ell(E',g) = \int_{\omega_g(E')}^{\omega_{g-1}(E')} d\omega \left[1 + 2\gamma(E')\,\omega + \gamma^2(E') \right]^{-1/2} P_\ell(\omega) \tag{16}$$

so that

$$X_{1,\ell}(E',g) = \int_{\omega_g(E')}^{\omega_{g-1}(E')} d\omega \; \frac{1 + \gamma(E')\,\omega}{\left[1 + 2\gamma(E')\,\omega + \gamma^2(E') \right]^{1/2}} \; P_\ell(\omega) \tag{17}$$

can be expressed by

$$\begin{aligned} X_{1,\ell}(E',g) &= Y_\ell(E',g) \\ &+ \frac{\gamma(E')}{2\ell+1} \left[(\ell+1)\, Y_{\ell+1}(E',g) + \ell\, Y_{\ell-1}(E',g) \right] . \end{aligned} \tag{18}$$

With the use of the properties of the Legendre polynomials it is possible to show that functions $Y_\ell(E',g)$ satisfy the recurrence relation, for $\ell \geqq 0$,

$$(2\ell+3)\, Y_{\ell+1}(E',g) = (1-\delta_{0,\ell})\,(1-2\ell)\, Y_{\ell-1}(E',g) - (2\ell+1)$$

$$\times \left[\frac{1}{\gamma(E')} + \gamma(E') \right] Y_\ell(E',g) + \frac{1}{\gamma(E')}$$

$$\times \left\{ [1 + 2\gamma(E')\,\omega + \gamma^2(E')]^{1/2}\, [P_{\ell+1}(\omega) - P_{\ell-1}(\omega)] \right\} \Bigg|_{\omega_g(E')}^{\omega_{g-1}(E')} \tag{19}$$

which can be used together with the initial value

$$Y_0(E',g) = \frac{1}{\gamma(E')} \left[1 + 2\gamma(E')\,\omega + \gamma^2(E') \right]^{1/2} \Bigg|_{\omega_g(E')}^{\omega_{g-1}(E')} \tag{20}$$

in order to calculate the functions $Y_\ell(E',g)$ required in Eq. (18) to establish functions $X_{1,\ell}(E',g)$. It is apparent that the recurrence relation expressed by Eq. (19) is not adequate in the limits $\gamma(E') >> 1$ and $\gamma(E') << 1$. In these cases, an alternative treatment becomes necessary. For $\gamma(E') >> 1$ we can use the representation [9]

$$\left[1 + 2\gamma(E')\,\omega + \gamma^2(E') \right]^{-1/2} = \sum_{m=0}^{\infty} (-1)^m \left[\frac{1}{\gamma(E')} \right]^{m+1} P_m(\omega) \quad , \tag{21}$$

valid for $\gamma(E') > 1$, in Eq. (17), obtaining the series

$$X_{1,\ell}(E',g) = \sum_{m=0}^{\infty} (-1)^m\, S_{m,\ell}(E',g)$$

$$\times \left[\left(\frac{m+2}{2m+3} \right) - \left(\frac{m}{2m-1} \right) \gamma^2(E') \right] \left[\frac{1}{\gamma(E')} \right]^{m+1} \tag{22}$$

where

$$S_{m,\ell}(E',g) = \int_{\omega_g(E')}^{\omega_{g-1}(E')} d\omega\, P_m(\omega)\, P_\ell(\omega) \quad . \tag{23}$$

Clearly, $S_{m,\ell}(E',g) = S_{\ell,m}(E',g)$. Moreover, it can be shown with the help of the properties of the Legendre polynomials that for $m \neq \ell$

$$[\, m(m+1) - \ell(\ell+1)\,]\, S_{m,\ell}(E',g) = \Big\{ \frac{m(m+1)}{2m+1} P_\ell(\omega)\, [\, P_{m+1}(\omega) - P_{m-1}(\omega)\,]$$

$$- \frac{\ell(\ell+1)}{2\ell+1} P_m(\omega)\, [\, P_{\ell+1}(\omega) - P_{\ell-1}(\omega)\,] \Big\} \Big|_{\omega_g(E')}^{\omega_{g-1}(E')} \tag{24}$$

and for $m = \ell$

$$(2\ell+3)\, S_{\ell+1,\ell+1}(E',g) = (2\ell+1)\, S_{\ell,\ell}(E',g)$$

$$+ \Big\{ \frac{\ell+2}{2\ell+3} [\, P_{\ell+2}(\omega) - P_\ell(\omega)\,]\, P_{\ell+1}(\omega) - \frac{\ell}{2\ell+1} \tag{25}$$

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

with

$$S_{0,0}(E',g) = \omega_{g-1}(E') - \omega_g(E') \quad . \tag{26}$$

For $\gamma(E') << 1$ the representation [9]

$$[\, 1 + 2\gamma(E')\,\omega + \gamma^2(E')\,]^{-1/2} = \sum_{m=0}^{\infty} (-1)^m\, \gamma^m(E')\, P_m(\omega) \quad , \tag{27}$$

valid for $0 \leq \gamma(E') < 1$, when substituted into Eq. (17), gives the series

$$X_{1,\ell}(E',g) = \sum_{m=0}^{\infty} (-1)^m S_{m,\ell}(E',g) \left[\left(\frac{m-1}{2m-1} \right) - \left(\frac{m+1}{2m+3} \right) \gamma^2(E') \right] \gamma^m(E'). \quad (28)$$

Equations (22) and (28) can therefore be used to calculate functions $X_{1,\ell}(E',g)$ efficiently in situations where the stability of the recurrence relation, Eq. (19), is in danger.

3. FINAL CONSIDERATIONS

The expressions given in the preceding section enable us to evaluate without recourse to numerical integration the angular integrals found in the generation of the isotropic and linearly anisotropic components of transfer matrices for elastic and discrete inelastic scattering. Since the representations of $f_x(E',\omega)$ in Legendre polynomials supplied by the ENDF/B library can include up to 21 terms in the expansion, depending on the element and the value of the initial energy, the numerical integration technique calls for quadratures of order > 10 in the execution of angular integration, requiring evaluation of the Legendre polynomials for each of the nodes of the selected quadrature, while the technique proposed here requires evaluation of the Legendre polynomials only in the integration limits. Moreover, in the numerical integration technique, the results obviously depend on the quadrature selected.

After the angular integration treated in detail in this work the generation of the isotropic and linearly anisotropic components of transfer matrices for elastic and discrete inelastic scattering involves the integration over energy shown in Eq. (11). There are in principle several ways of carrying out this integration, varying from linear approximations like those used by the MC^2 and MC^2-2 codes in the ultra- and hyperfine structures, respectively, to gaussian quadratures such as those used in the NJOY system. Our purpose in implementing the method is to use the trapezoidal rule in the grid obtained by adding the discrete structure utilized in the ENDF/B library to store $\sigma_x(E')$ (in the case of resolved resonances, the grid obtained in the reconstruction process will be used) and $f_x(E',\ell)$ with the integration limits of Eq. (11), and we believe this will minimize the number of necessary interpolations without sacrificing the accuracy of the final result.

The technique described here will shortly be implemented so that it will be possible to make a specific evaluation of its use in comparison with the other techniques currently utilized in the generation of transfer matrices for elastic and discrete inelastic scattering.

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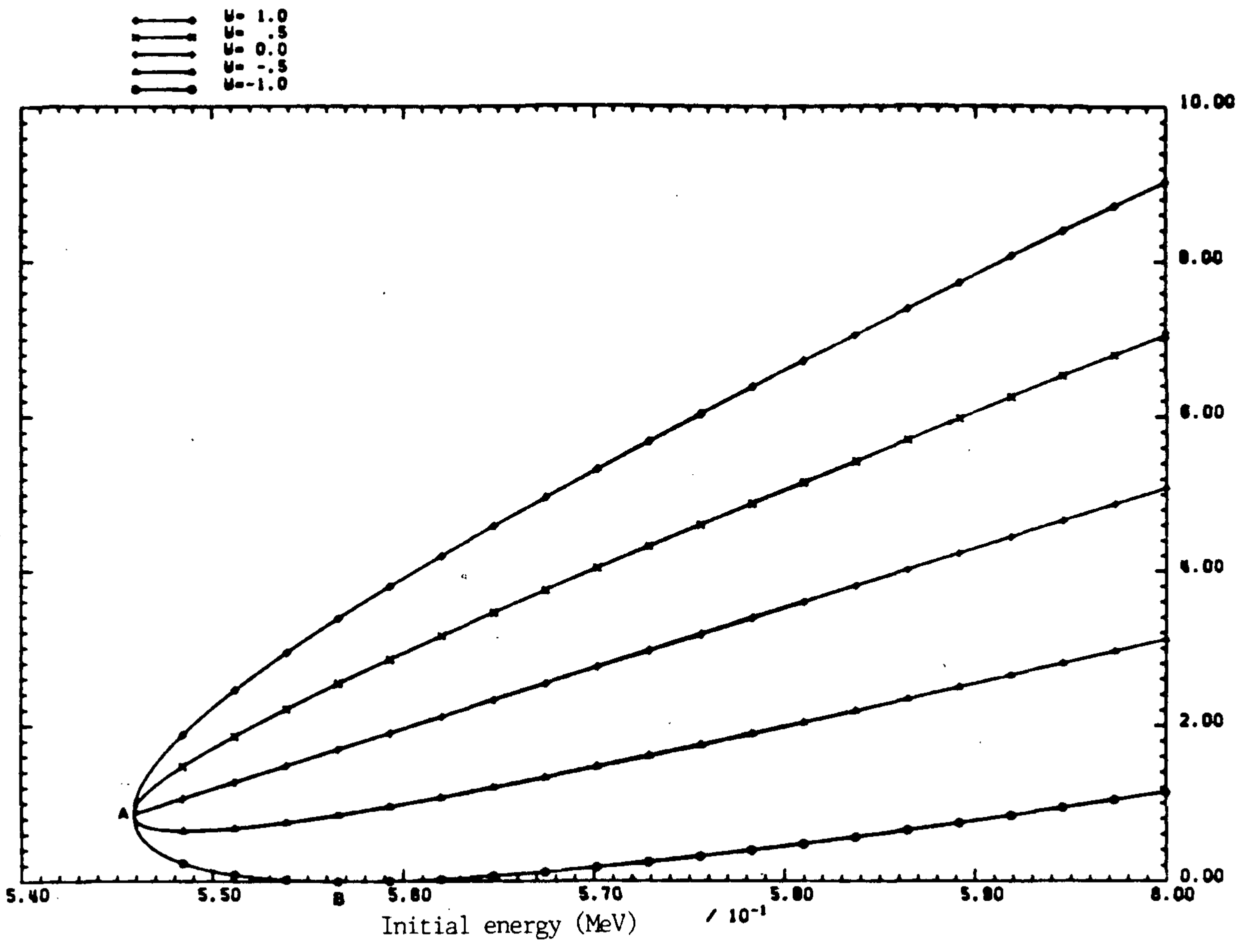

Fig. 1. Relation between final energy E and initial energy E' for discrete inelastic scattering involving the first excitation level of ^7Li.