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MODIFICATION OF THE SUPERTOG PROGRAM APPLIED TO LIBRARIES WITH TABULATED ELASTIC-SCATTERING ANISOTROPY DENSITIES

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MODIFICATION OF THE SUPERTOG PROGRAM APPLIED TO LIBRARIES WITH TABULATED ELASTIC-SCATTERING ANISOTROPY DENSITIES

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ABSTRACT

In calculating the matrix for intergroup elastic-scattering transitions by the SUPERTOG program, it is necessary that the data on the anisotropy of the elastic scattering be given in terms of the coefficients for a Legendre polynomial expansion of the density function. However, for all the material in the ENDL library and for some of the material in ENDF/B-IV, the information on the scattering anisotropy is given in the form of tabulated values of the actual density function. Existing versions of the SUPERTOG program cannot be used for these materials.

We have developed a modification of the SUPERTOG program which enables us to calculate the elastic-scattering matrix whichever of the two ways the anisotropy is given. With this method, which is based on an approximation by means of orthonormal polynomials, it is possible to calculate the coefficients in the Legendre polynomial expansion of the density function during the operation of the actual program. In fact, this procedure takes less than 15% of the total running time of SUPERTOG.

1. INTRODUCTION

The SUPERTOG program [1] is one of the widely used methods for preparing data for multigroup neutron transport calculations. The program gives the following information:

(a) Scattering cross-sections averaged over energy groups; and

(b) Matrices for intergroup transitions resulting from elastic and inelastic scattering and (n,2n) reactions.

For calculating the elastic-scattering transition matrix, the program needs the group averaged elastic-scattering cross-sections and data on the anisotropy in the centre-of-mass system. In the ENDF/B format files [2], the information on the scattering anisotropy is usually given in one of two ways: as tabulated values of the function $p(\mu,E)$ for the probability density of the scattering of a neutron with energy E at an angle θ ($\mu = \cos\theta$) or as the coefficients $f_\ell(E)$ in the expansion of the function $p(\mu,E)$ in the Legendre polynomials $L_\ell(\mu)$:

$$p(\mu, E) = \sum_{\ell=0}^{N} \frac{2\ell+1}{2} f_\ell(E) L_\ell(\mu) \qquad (1)$$

where N is the optimal order for truncating the series.

The existing versions of the SUPERTOG program can calculate the elastic-scattering group transition matrix only when the coefficients $f_\ell(E)$ are given in the library of initial nuclear physical constants. However, for all the material in the ENDL library and for some of the material in ENDF/B-IV, the elastic-scattering anisotropy is given in the form of tabulated values of the function $p(\mu,E)$.

2. FORMULATION OF THE PROBLEM

The need therefore arises to modify the SUPERTOG program so that the elastic-scattering matrix can be calculated for either of the two ways in which the anisotropy information may be given. This means that for given sets

$$\{\mu_i\}, \quad \{p(\mu_i, E)\} \quad i = 1, 2, \ldots, m$$

corresponding to some fixed energy E, we have to find the order N and the set of coefficients

$$\{ f_\ell(E) \}_{\ell = 0, 1, \ldots, N}$$

which, when substituted into the right-hand side of Eq. (1), would reconstruct the tabulated values of $p(\mu, E)$ with an accuracy no worse than that of the original data.

At least three approaches to the solution of the overall problem are possible:

(a) To change the calculation algorithim in SUPERTOG and thus to get the possibility of working directly with the tabulated values of the function $p(\mu, E)$;

(b) To carry out expansion of the function $p(\mu, E)$ in terms of Legendre polynomials [i.e. to calculate the coefficients $f_\ell(E)$] during the running of the SUPERTOG program;

(c) To prepare beforehand a version of the library in which the tables of the function $p(\mu, E)$ are replaced by the corresponding coefficients $f_\ell(E)$.

We have developed a modification of the SUPERTOG program in which the coefficients $f_\ell(E)$ are calculated during the running of the program itself inside the algorithim for calculating the elastic-transition matrix.

3. METHODS OF SOLUTION

3.1. The coefficients $f_\ell(E)$ can be calculated directly by numerical integration. Since the Legendre polynomials are orthogonal, we have in fact from Eq. (1) that

$$f_\ell(E) = \int_{-1}^{1} p(\mu, E) L_\ell(\mu) \, d\mu \,, \quad \ell = 0, 1, \ldots, N \tag{2}$$

here,

E is the neutron energy in electron volts,

$\mu = \cos\theta$, where θ is the scattering angle in the centre-of-mass system,

$L_\ell(\mu)$ is the Legendre polynomial of order ℓ, and

$p(\mu, E)$ is the probability density for elastic scattering of a neutron with energy E at an angle θ, where $\theta = \cos^{-1}\mu$.

In view of the severe non-linearity of the higher-order polynomials $L_\ell(\mu)$, this approach requires the use of a close numerical-integration grid and leads - for reasonable accuracy in the estimates of Eq. (2) - to large expenditures of machine time, considerably greater than the normal calculation time in the SUPERTOG program.

3.2. Using the values of the sets from section 2, we can write expression (2) in the form

$$f_\ell(E) = \sum_{i=1}^{m-1} \int_{\mu_i}^{\mu_{i+1}} p(\mu, E)\, L_\ell(\mu)\, d\mu \qquad (3)$$

We shall denote the coefficients in the expansion of the Legendre polynomial $L_\ell(\mu)$ by $b_j^{(\ell)}$:

$$L_\ell(\mu) = \sum_{j=0}^{\ell} b_j^{(\ell)} \mu^j . \qquad (4)$$

We shall further assume that in the interval $[\mu_i, \mu_{i+1}]$, $i = 1, 2, \ldots, m-1$, the values of the function $p(\mu, E)$ are calculated from the linear interpolation model

$$p(\mu, E) = \gamma_i \mu + \delta_i \,, \quad \mu_{i+1} \le \mu \le \mu_i \qquad (5)$$

where

$$\gamma_i = \frac{p(\mu_{i+1}, E) - p(\mu_i, E)}{\mu_{i+1} - \mu_i}$$

and

$$\delta_i = \frac{\mu_{i+1}\, p(\mu_i, E) - \mu_i\, p(\mu_{i+1}, E)}{\mu_{i+1} - \mu_i}$$

Then, using Eqs (4) and (5), we get from expression (3) that

$$f_\ell(E) = \sum_{i=1}^{m-1} \sum_{j=0}^{\ell} b_j^{(\ell)} \int_{\mu_i}^{\mu_{i+1}} (\gamma_i \mu^{j+1} + \delta_i \mu^j)\, d\mu .$$

After integration and some cumbersome but elementary alegbra we arrive at the following expression for the coefficients $f_\ell(E)$:

$$f_\ell(E) = \sum_{\substack{j=\mathrm{mod}(\ell,2) \\ \text{step } 2}}^{\ell} \frac{b_j^{(\ell)}}{j+2} \left[p(1,E) + (-1)^j p(-1,E) \right] +$$

$$+ \sum_{\substack{j=\mathrm{mod}(\ell,2) \\ \text{step } 2}}^{\ell} \frac{b_j^{(\ell)}}{(j+1)(j+2)} \sum_{i=1}^{m-1} \frac{\mu_{i+1} p(\mu_i,E) - \mu_i p(\mu_{i+1},E)}{\mu_{i+1} - \mu_i} \left(\mu_{i+1}^{j+1} - \mu_i^{j+1} \right),$$

where the summation over the index ℓ takes into account the fact that the $L_\ell(\mu)$ are even functions.

Despite the fact that libraries of nuclear physical constants are in fact designed to use linear interpolation for getting the values of $p(\mu, E)$ in the grid intervals $\{\mu_i\}$ the accuracy of the numerical approximation obtained by this method is unsatisfactory. This seems to be the result of the loss of significant figures that occurs when working with coefficients $b_j^{(\ell)}$ which vary in sign and have a large absolute value.

3.3. The third approach to the calculation of $f_\ell(E)$ consists in using a special class of orthonormal polynomials [3-5]. This approach reduces to two steps:

3.3.a. We construct [3] the set of polynomials $\{P_\ell(\mu)\}_{\ell=0,1,\ldots,m-1}$ which are orthonormalized in the point set $\{\mu_i\}_{i=1,2,\ldots,m}$ with weights $\{w_i\}$, where

$$w_1 = c\,(\mu_2 - \mu_1)$$

$$w_i = c\,(\mu_{i+1} - \mu_{i-1}), \quad i = 2, 3, \ldots, m-1$$

$$w_m = c\,(\mu_m - \mu_{m-1})$$

and the constant c is determined from the condition for normalization of the density function $p(\mu, E)$,

$$\int_{-1}^{1} p(\mu, E)\, d\mu = 1$$

This choice of weights allows for the fact that the grid $\{\mu_i\}$, is non-uniform and also takes into account the linearity of the interpolation model from which the values of $p(\mu, E)$ are calculated in the grid intervals. We can now express the anisotropy function as

$$p(\mu, E) = \sum_{j=0}^{N} a_j(E)\, P_j(\mu) \tag{6}$$

where $N \leqslant m-1$ and the coefficients a_j are calculated from the equation

$$a_j(E) = \sum_{i=1}^{m} p(\mu_i, E)\, \omega_i\, P_j(\mu_i).$$

3.3.b. We now have to transform the coefficients $\{a_j\}$ into the $\{f_\ell\}$ from Eq. (1). As expected, this transformation is most accurate and stable from the point of view of numerical calculations when it is made in the orthonormal basis $\{P_j\}$. We therefore expand the Legendre polynomials in this basis:

$$L_\ell(\mu) = \sum_{j=0}^{\ell} c_j^{(\ell)}\, P_j(\mu) \tag{7}$$

where

$$c_j^{(\ell)} = \sum_{i=1}^{m} L_\ell(\mu_i)\, \omega_i\, P_j(\mu_i) \tag{8}$$

Substituting Eqs (6) and (7) into expression (1), we get the relationship

$$\sum_{j=0}^{N} a_j(E)\, P_j(\mu) = \sum_{j=0}^{N} \frac{2j+1}{2}\, f_j(E) \sum_{\kappa=0}^{j} c_\kappa^{(j)}\, P_\kappa(\mu)$$

from which we can easily derive a triangular system of linear equations in the unknown coefficients $f_j(E)$.

$$f_i(E) = \frac{2}{(2i+1)\,c_i^{(i)}} \left[a_i(E) - (1-\delta_{iN}) \sum_{j=i+1}^{N} f_j(E)\, a_i^{(j)} \right] \qquad (9)$$

where $i = N, N-1, \ldots, 2, 1, 0.$

4. CHOICE OF OPTIMUM APPROXIMATION ORDER

As we have already mentioned, a linear interpolation model was provided in the libraries for the preparation of evaluated data on the anisotropy of elastic scattering. In other words, the data were normalized so that the normalization condition

$$f_0(E) = \int_{-1}^{1} p(\mu, E)\, d\mu = 1$$

was satisfied most accurately for numerical integration by the trapezoidal method. Thus, the condition for the coefficient $f_0(E)$ to be close to unity is also the criterion for the expansion to be close to the linear model for the interpolation of the function $p(\mu, E)$.

On the other hand, to obtain a more accurate approximation by Legendre polynomials it is necessary to include terms of a comparatively high order in the expansion. Oscillations then begin to occur in the approximating curves as a result of the limited accuracy of the numerical calculations. In particular, this can lead to significant deviations of $f_0(E)$ from unity.

To damp out the oscillations, the algorithim includes the addition of a grid $\{\mu_i\}$ of intermediate points. The values of $p(\mu, E)$ at these points are calculated by linear interpolation of the data in the original grid. The number and positions of the intermediate points are chosen so that not only are the oscillations damped but the uniformity of the grid is improved. The condition is imposed that the maximum absolute deviation of $f_0(E)$ from unity should not exceed 0.005.

Next, from the set of values N satisfying this criterion, the choice of the optimum order is made. The criterion is that the following product should be a minimum:

$$CHI(N) * EYMAX(N) * ED(N)$$

where CHI(N) is the value of χ^2 normalized to one degree of freedom;

EYMAX(N) is the maximum relative deviation of the approximating series from the initial data at the grid points (initial or supplementary);

ED(N) is the maximum absolute deviation at the same points.

5. PROGRAMING DETAILS

Our version of the SUPERTOG program which accepts both forms of the information on elastic-scattering anisotropy in the centre-of-mass system includes:

(a) The necessary changes in the SUPERTOG-4 program package, NEA DATA BANK - 1978 version;

(b) The LTTAS1 package, which calculates the coefficients f_ℓ (E) in the expansion of the function $p(\mu,E)$.

The changes in SUPERTOG concern the TRANS, GADD and TMF4 modules. A sub-program TAB1S is added to arrange proper storage of the library data on the anisotropy.

The LTTAS1 package is only called when it is necessary to calculate the elastic scattering matrix and if the value of the parameter LTT in the ENDF/B format file is equal to 2 - corresponding to tabulated density functions. If these conditions are satisfied, the TMF4 sub-program of the SUPERTOG package calls on LTTAS1, which consists of the following modules:

5.1. LTTAS1 - the control module of the package. This checks the initial anisotropy data, prints control information on the Legendre approximation process and stores the calculated expansion coefficients in the SUPERTOG COMMON area.

5.2. ORNINT - controls the orthonormalized and Legendre approximation processes.

5.3. WEIGHT, FLINT - calculate the weighting coefficients and carry out linear interpolation of the function $p(\mu,E)$.

5.4. APPRO1, PREPF1, ORTHN1 [3, 5] - calculate the coefficients of the orthonormalized approximation (6).

5.5. LORTHB - calculates the coefficients of the Legendre polynomial expansion in terms of the polynomials of the orthonormalized basis $\{P_j(\mu)\}$.

5.6. CRIT - makes the choice of the optimum order N for the approximation by the Legendre series.

5.7. LEGEX - solves the triangular system of linear equations (9) and finds the coefficients $f_\ell(E)$.

5.8. OPTHNL - calculates the values of the Legendre polynomials by a three-term recursive method.

5.9. TELSCL - calculates the sum on the right-hand side of Eq. (1) by the telescoping method [5, 6].

5.10. ERR1 - prints information on the imposed limitations in the order of approximation N and on the errors in the operation of the LTTAS1 package.

6. DISCUSSION OF RESULTS

In accordance with the requirements of the algorithms followed in SUPERTOG, the order of the Legendre polynomial expansion of the function $p(\mu,E)$ should not exceed 30 (not more than 31 coefficients, including the zeroth). The special attention given to the problem of making the coefficient $f_o(E)$ as close to unity as possible is due to the fact that in SUPERTOG this value is taken necessarily to be equal to unity.

Table 1 shows for comparison purposes the results of approximating the function $p(\mu,E)$ by methods 3.2 (direct use of the linear interpolation model) and 3.3 (approximation by orthonormalized polynomials). For both methods, the appropriate optimum expansion orders have been chosen. The advantage of the second approach is fairly clear.

Table 2 gives the tabulated and reconstructed values of the density function for ^{235}U when E = 4.0 MeV. The second column lists the values calculated from $f_\ell(E)$ coefficients taken from the ENDF/B-IV Standard library. The next column contains the values tabulated in the ENDL library

and the final column the values reconstructed from the $f_\ell(E)$ coefficients obtained at the output of our LTTAS1 package. It is once again clear that the values in the fourth column are more accurate.

We may note in conclusion that unsatisfactory results in the numerical approximation of the density function $p(\mu,E)$ (i.e. large absolute or relative deviations, negative values and so on) are observed in two cases:

(a) The function $p(\mu,E)$ changes fairly rapidly in the interval $-1 \leqslant \mu \leqslant 1$, and its tabulated values in the library are given at fewer than 10 points. It may be assumed in this case that the linear interpolation model gives a poor description of the scattering process;

(b) The function is given at the points of a fairly close grid over the same interval but the actual values of the function differ from one another by 4–5 orders of magnitude. This form of numerical problem is more difficult to avoid, since it arises from the limited accuracy with which numbers are represented in the computer. It helps to some extent to get proper choice of the system of polynomials in which the function is expanded. This in fact explains the higher accuracy obtained when working with the LTTAS1 package.

Table 1.

Comparison of the accuracy of the approximation for the density function $p(\mu,E)$ with direct use of linear interpolation (method 3.2) and in the basis of orthonormalized polynomials (method 3.3) for the isotope ^{239}Pu from the ENDL library: E = 1.46 MeV.

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*/ 0.43874 -1 means 0.43874×10^{-1}.

Table 1

Method		3.2.		3.3.	
Optimum order of expansion		17		30	
Value $f_0(E)$		0.100000 + 1		0.100029 + 1	
μ	$P(\mu, E)$ Libr.	$\left\|\frac{\Delta p}{p}\right\|$ %	$P(\mu, E)$ Approx.	$\left\|\frac{\Delta p}{p}\right\|$ %	$P(\mu, E)$ Approx.
-1.00	0.43874 - 1+	89	0.47923 - 2	25	0.33087 - 1
-0.9499	0.43874 - 1	97	0.97454 - 3	35	0.59388 - 1
-0.85	0.21987 - 1	280	0.83719 - 1	43	0.31569 - 1
-0.75	0.21987 - 1	283	-0.40303 - 1	53	0.33736 - 1
-0.65	0.21987 - 1	120	0.48501 - 1	29	0.15700 - 1
-0.55	0.21987 - 1	414	0.11306	12	0.19369 - 1
-0.45	0.21987 - 1	395	-0.65050 - 1	37	0.30176 - 1
-0.35	0.32880 - 1	250	-0.49572 - 1	30	0.22862 - 1
-0.25	0.43874 - 1	234	0.14642	27	0.55875 - 1
-0.15	0.65861 - 1	93	0.12714	21	0.51920 - 1
-0.05	0.65861 - 1	173	-0.48380 - 1	16	0.76487 - 1
0.05	0.43874 - 1	112	-0.53558 - 2	28	0.31322 - 1
0.15	0.43874 - 1	368	0.20517	61	0.70449 - 1
0.25	0.17590	27	0.22315	8	0.16133
0.35	0.33480	58	0.13904	2	0.34113
0.45	0.33480	8	0.30890	10	0.29970
0.55	0.21987	89	0.41477	16	0.25489
0.65	0.21987	16	0.18452	22	0.26843
0.75	0.97642	14	0.84258	8	0.89641
0.85	0.93244	9	0.10134 + 1	10	0.83464
0.90	0.27384	213	-0.31159	31	0.35870
0.91	0.21987	293	-0.42475	34	0.29567
0.92	0.16490	300	-0.33005	59	0.26240
0.93	0.32880	73	0.87734 - 1	3	0,31815
0.94	0.93244	5	0.97680	32	0.62662
0.95	0.17590 + 1	43	0.25244 + 1	13	0.15336 + 1
0.96	0.31781 + 1	56	0.49640 + 1	14	0.36279 + 1
0.97	0.74156 + 1	16	0.85828 + 1	4	0.76859 + 1
0.98	0.14891 + 2	8	0.13730 + 2	4	0.14277 + 2
0.99	0.22287 + 2	6	0.20828 + 2	1	0.22594 + 2
1.00	0.27783 + 2	9	0.30379 + 2	0.4	0.27681 + 2

Table 2.

Tabulated and reconstructed values of the density function $p(\mu,E)$ for the isotope ^{235}U with E = 4.0 MeV according to the data from the ENDF/B-IV Standard and ENDL libraries.

Table 2

μ	$P(\mu, E)$		
	Reconstructed from coefficients obtained from ENDF/B-IV Standard	Tabulated values ENDL	Reconstructed from coefficients obtained with LTTAS1
-1.00	0.58775 - 1	0.17310	0.17250
-0.95	0.11209 - 1	0.13710	0.13769
-0.85	0.13624 - 1	0.71130 - 1	0.76982 - 1
-0.75	0.64014 - 1	0.44120 - 1	0.58130 - 1
- 0.65	0.97326 - 1	0.35020 - 1	0.27955 - 1
-0.55	0.94952 - 1	0.35020 - 1	0.36169 - 1
-0.45	0.70763 - 1	0.49120 - 1	0.49684 - 1
-0.35	0.49304 - 1	0.66130 - 1	0.62925 - 1
-0.25	0.48220 - 1	0.71130 - 1	0.71519 - 1
-0.15	0.70514 - 1	0.93140 - 1	0.94942 - 1
-0.05	0.10669	0.12000	0.11409
0.05	0.14282	0.15510	0.16374
0.15	0.16856	0.19910	0.18378
0.25	0.17974	0.19910	0.20866
0.35	0.17359	0.15110	0.13650
0.45	0.14206	0,13310	0.15038
0.55	0.79725 - 1	0.10600	0.84804 - 1
0.65	0.38667 - 1	0.11500	0.14523
0.75	0.28380	0.33210	0.39201
0.85	0.16285 + 1	0.12600 +1	0.12768 +1
0.95	0.60632 + 1	0.54220 +1	0.54024 +1
1.00	0.10635 + 2	0.10200 +2	0.10200 +2

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