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LEGENDRE-SERIES DEVELOPMENT OF THE ANISOTROPY DENSITY OF NEUTRON ELASTIC SCATTERING BY MEANS OF CUBIC SPLINES

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ABSTRACT

The Legendre-series coefficients of the anisotropy density of neutron elastic scattering are computed starting from tabulated data and using the basis of natural cubic splines. The method is implemented and incorporated in the SUPERTOG package. Processing results are reported and compared with previous ones.

INTRODUCTION

The anisotropy density of scattering is usually represented by means of the Legendre-series coefficients. This is being done despite the well-known fact that polynomials are not always suitable for the approximation of this class of functions. Nevertheless, as Legendre series are derived when the problem is analytically solved and as there exists a number of computer codes which solve the same problem numerically on the basis of a polynomial model, the search for effective numerical procedures converting tabulated data into a set of Legendre coefficients cannot as yet be considered out-of-date.

In ref. [1] a method is proposed which uses a basis of special-class polynomials to represent both the anisotropy and the Legendre polynomials. The Legendre coefficients are then derived from these presentations. The procedure is programmed and incorporated in the SUPERTOG package which prepares

multigroup constants for the solution of neutron transfer problems.

When this modified SUPERTOG version was used to prepare the L26P3S34 library[2] , however, a limited number of cases was observed where unsatisfactory fits were computed. For some materials at certain energies and angles the anisotropy-density function restored by means of the Legendre coefficients was deviating considerably from table data and even reaching negative values.

In the present paper a similar method is described. It differes from that of [1] by the use of natural cubic spline basis instead of special-class polynomials. Input data and output results are, as before, tabulated anisotropy-density values and Legendre coefficients respectively. Again, the procedure is implemented and incorporated in SUPERTOG.

FORMULATION OF PROBLEM

Let the elastic-scattering anisotropy data in the centre-of-mass system be given in the form of tabulated values of the function $p(\mu, E)$, i.e. the probability density of scattering a neutron of energy E at an angle θ , $\mu = \cos\theta$. To develop in a Legendre-polynomial series will then mean to find the order N and the coefficients $\{f_\ell(E)\}$ of the series

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

at given sets

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

where $L_\ell(\mu)$ is a Legendre polynomial of order ℓ. It is requested that (1) restore with greatest possible accuracy the input set $\{p(\mu_i, E)\}$.

METHOD OF SOLUTION

Due to the orthogonality of $L_\ell(\mu)$ we obtain from eq.(1)

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

and

$$f_\ell(E) = \sum_{i=1}^{m-1} \int_{\mu_i}^{\mu_{i+1}} p(\mu, E)\, L_\ell(\mu)\, d\mu \,, \quad \ell = 0, 1, \ldots, N \,. \tag{2}$$

Let in each interval $[\mu_i, \mu_{i+1}]$, $i = 1, 2, \ldots, m-1$ the function $p(\mu, E)$ be approximated by a natural cubic spline with coefficients b_i, c_i, d_i,

$$p(\mu, E) = p_i + b_i(\mu - \mu_i) + c_i(\mu - \mu_i)^2 + d_i(\mu - \mu_i)^3$$

where $\mu \in [\mu_i, \mu_{i+1}]$ and $p_i = p(\mu_i, E)$.

Accordingly, let

$$L_\ell(\mu) = L_{\ell,i} + f_{\ell,i}(\mu - \mu_i) + g_{\ell,i}(\mu - \mu_i)^2 + h_{\ell,i}(\mu - \mu_i)^3$$

be the cubic-spline approximation of the polynomial $L_\ell(\mu)$, where the coefficients are $f_{\ell,i}$, $g_{\ell,i}$, $h_{\ell,i}$, and $L_{\ell,i}$ denotes $L_\ell(\mu_i)$.

We can now rewrite eq.(2) in the form

$$\begin{aligned} f_\ell(E) &= \sum_{i=1}^{m-1} \int_{\mu_i}^{\mu_{i+1}} p(\mu, E)\, L_\ell(\mu)\, d\mu \\ &= \sum_{i=1}^{m-1} \int_{\mu_i}^{\mu_{i+1}} d\mu \left[p_i + b_i(\mu - \mu_i) + c_i(\mu - \mu_i)^2 + d_i(\mu - \mu_i)^3 \right] \\ &\quad \cdot \left[L_{\ell,i} + f_{\ell,i}(\mu - \mu_i) + g_{\ell,i}(\mu - \mu_i)^2 + h_{\ell,i}(\mu - \mu_i)^3 \right] \\ &= \sum_{i=1}^{m-1} \sum_{k=0}^{6} A^{(k)}_{\ell,i} \int_{\mu_i}^{\mu_{i+1}} (\mu - \mu_i)^k\, d\mu \,, \end{aligned}$$

where

$$\begin{aligned} A^{(0)}_{\ell,i} &= p_i L_{\ell,i} \\ A^{(1)}_{\ell,i} &= p_i f_{\ell,i} + b_i L_{\ell,i} \\ A^{(2)}_{\ell,i} &= p_i g_{\ell,i} + b_i f_{\ell,i} + c_i L_{\ell,i} \\ A^{(3)}_{\ell,i} &= p_i h_{\ell,i} + b_i g_{\ell,i} + c_i f_{\ell,i} + d_i L_{\ell,i} \\ A^{(4)}_{\ell,i} &= b_i h_{\ell,i} + c_i g_{\ell,i} + d_i f_{\ell,i} \\ A^{(5)}_{\ell,i} &= c_i h_{\ell,i} + d_i g_{\ell,i} \\ A^{(6)}_{\ell,i} &= d_i h_{\ell,i} \,. \end{aligned}$$

Integrating the previous expression we obtain the coefficients sought for

$$f_\ell(E) = \sum_{i=1}^{m-1} \sum_{k=0}^{6} \frac{\Delta_i^{k+1}}{k+1} A_{\ell,i}^{(k)} \tag{3}$$

where $\Delta_i = \mu_{i+1} - \mu_i$, $i = 1, 2, \ldots, m-1$.

The optimum order N is defined as follows. The coefficients $f_\ell(E)$ are computed up to ℓ_{max}=min(30,m-1). The set $N=[0,\ell_{max}]$ is investigated and a subject $S \subseteq N$ is defined for which the values restored

$$\sum_{\ell=0}^{6} \frac{2\ell+1}{2} f_\ell(E) L_\ell(\mu) \ , \ s \in S$$

are non-negative. Then N is selected from the condition

$$(\min_s \max_i \Delta_i^{(s)} \delta_i^{(s)}) \cdot \chi^2_s \rightarrow \min$$

where χ^2_s is the chi-square normalized to one degree of freedom, $\Delta_i^{(s)}$ and $\delta_i^{(s)}$ are respectively the absolute and the relative deviation at point i for order of approximation s.

If S is an empty set, then the criterion is modified to test all the orders $\ell \in [0, \ell_{max}]$.

IMPLEMENTATION

The program implementation takes into account the requirement that the method should work in the SUPERTOG environment, using evaluated data in the ENDF/B format. Surely, the set of routines is also able to run outside the SUPERTOG-imposed limits. More essential are, however, their relations with data structure in library files. To damp down possible oscillations of the fitting function at intergrid points the algorithm adds a point to the middle of each interval $[\mu_i, \mu_{i+1}]$, i = 1,2,...,m-1. Library files are usually built in a way that the normalizing relation

$$1 = f_0(E) = \sum_{i=1}^{m-1} \int_{\mu_i}^{\mu_{i+1}} P(\mu, E)\, d\mu$$

be satisfied for the case of linear interpolation between each

pair of grid points. Hence, these additional points should be given values

$$p(\mu, E) = \frac{1}{2}\left[p(\mu_i, E) + p(\mu_{i+1}, E)\right] .$$

Therefore, the vicinity of $f_0(E)$ to unity is a measure of validity for the linear interpolation model. At a preliminary stage of testing the method we used this property as a quality control of the spline approximation. Moreover, we found it more appropriate to fit separately the two functions $p(\mu, E)$ and $L_\ell(\mu)$ rather than their product $p(\mu, E)\, L_\ell(\mu)$.

Our SUPERTOG version in which the algorithm outlined is implemented includes:

(a) the necessary modifications of the SUPERTOG package, version NEA-DATA-BANK (1978). These modifications practically coincide with those introduced into the package for the orthonormal-polynomial basis [1] ;

(b) the SPLINT subpackage which computes the coefficients $f_\ell(E)$ of eq.(1).

The SUPERTOG modifications affect subroutines TRANS, GADD and TMF4; to avoid collisions when reading in the library data on elastic-scattering anisotropy, a new TAB1S routine is added.

The SPLINT subpackage is only called when the computation of the elastic-scattering matrix is needed and, in that case, if and only if the LTT parameter of the ENDF/B input file equals 2 (this corresponds to tabulated values of the function of the probability density). When both conditions are satisfied, the TMF4 routine of SUPERTOG calls SPLINT which consists of the following modules:

1) LTTAS1 - a control subroutine;

2) SPLINT - computes the coefficients $f_\ell(E)$ according to (3);

3) CRIT - selects the optimum order N of the Legendre's fitting series;

4) PLX - calculates the values of $L_\ell(\mu)$ by means of the three-term recurrence;

5) TELSCL - computes the right-hand side of eq.(1) using the telescoping method;

6) SPLINE - carries out the natural cubic-spline approximation [3] .

DISCUSSION

Testing results are illustrated in Tables 1-4. The first three tables offer a comparison of precision reached when Legendre coefficients are computed in the orthonormal [1] vs spline bases. The ENDL material 7132 (iron) was processed at energies of.4,5 and 7 MeV. Table 4 shows the optimum orders N and the values of $f_0(E)$ for the same energies. We call here a "fit order" the maximum order of Legendre polynomial in the series. It should be noticed that, whatever the value computed of $f_0(E)$, SUPERTOG sets it to unity compulsorily. Hence, the same unit value is used to compute the optimum order N of series development.

The following conclusions may be made from the testing results. The orthonormal expansion method sometimes shows an instability manifested in linear fits of smooth but nonlinear functions. Moreover, for rapidly-changing functions it may lead to oscillations and even to negative probabilities. In these two cases the natural cubic spline method is the winner, although in general it ensures a lower precision because of stronger deviations from the linear interpolation model. This means that $f_0(E)$ may strongly differ from unity in the spline

Table 1

Restored function $p(\mu, E)$; material 7132 (Fe)

of ENDL, E = .4 MeV

μ	Library value	Orthonormal basis	$\frac{\Delta p}{p}$ %	Spline basis	$\frac{\Delta p}{p}$ %
-1.0	0.44500	0.32238	27.6	0.45160	-1.5
-0.7	0.40000	0.37567	6.1	0.40502	-1.3
-0.5	0.40000	0.41119	-2.8	0.39988	0.3
0.1	0.44500	0.50000	-12.4	0.45309	-1.8
1.0	0.71900	0.67762	5.8	0.73607	-2.4

Table 2

Restored function $p(\mu, E)$; material 7132 (Fe)

of ENDL, E = 5 MeV

μ	Library value	Orthonormal basis	$\frac{\Delta p}{p}$ %	Spline basis	$\frac{\Delta p}{p}$ %
-1.00	0.73128-1*	0.75361-1	-3.1	0.11354	-55.3
-0.85	0.36614-1	0.41267-1	-12.7	0.46629-1	-27.4
-0.50	0.91435-1	0.96385-1	-5.4	0.10180	-11.3
-0.35	0.12805	0.12695	0.7	0.12502	2.4
-0.30	0.12805	0.13108	-2.4	0.13017	-1.7
-0.10	0.91435-1	0.90433-1	1.1	0.11390	-24.6
0.15	0.36614-1	0.38198-1	-4.3	0.33107-1	9.6
0.30	0.36614-1	0.40742-1	-11.3	0.49516-1	-35.2
0.40	0.73128-1	0.93188-1	-27.4	0.13844	-83.3
0.70	0.95137	0.97714	-2.7	0.10471+1	-10.1
0.90	0.27411+1	0.27421+1	-0.4	0.28575+1	-4.2
1.00	0.47518+1	0.47540+1	-0.5	0.48401+1	-1.9

* 0.73128-1 means 0.73128×10^{-1}

Table 3

Restored function $p(\mu, E)$; material 7132 (Fe) of ENDL, E = 7 MeV

μ	Library value	Orthonormal basis	$\frac{\Delta p}{p}$ %	Spline basis	$\frac{\Delta p}{p}$ %
-1.00	0.33186-1	-0.79679		0.32305-1	2.7
-0.85	0.99458-2	-0.32855-1		0.15910-1	-60.0
-0.50	0.49779-1	0.43169		0.55005-1	-10.5
-0.15	0.82865-1	-0.67816-1		0.87012-1	-5.0
0.00	0.82865-1	-0.30687		0.89985-1	-8.6
0.35	0.33186-1	-0.29278		0.31886-1	3.9
0.60	0.16593	0.68407		0.26093	-57.3
0.80	0.11295+1	0.23506+1	-108.0	0.13061+1	-6.8
0.85	0.17893+1	0.29167+1	-63.0	0.19804+1	-10.7
0.95	0.53078+1	0.42503+1	19.9	0.54755+1	-3.2
1.00	0.86164+1	0.50243+1	47.7	0.86812+1	-0.8

Table 4

Values of optimum approximation orders N and zero-order coefficients $f_0(E)$ for the data of Tables 1-3

E/MeV/	Approximation order		zero-order coefficient $f_0(E)$	
	orthonormal	spline	orthonormal	spline
0.4	1	3	1.000000	0.998786
5.0	21	8	0.995492	0.980027
7.0	3	12	0.996811	0.979506

method. The orthonormal polynomials smooth the function being fitted, while the splines do not.

The study of the results for the same range of materials and energies where the weak points of the orthonormal method were detected leads to the conclusion that the same optimum criterion yields acceptable sets of coefficients for all the functions being fitted by means of the spline method. In particular, negative probabilities never occurred. On the other hand, however, "good" functions (which represent the majority) are better fitted by the orthonormal method.

In conclusion, we may recommend the splines in automated procedures of data preparation while, if one can control the optimum criterion during the calculations, the orthonormal polynomials are recommended instead.

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