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LUCAS HEIGHTS

GUNYA — A SYSTEM OF CODES FOR THE PREPARATION OF GYMEA CROSS SECTION DATA LIBRARIES

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ABSTRACT

A system of computer programmes called GUNYA is described which prepares multigroup cross section information suitable for input to the burnup code GYMEA.

CONTENTS

1. INTRODUCTION

A system of computer codes, called GUNYA has been developed to facilitate the rapid preparation of the large body of cross section data required to represent the effects of fission product poisoning in reactor fuel burnup. The code series has been enlarged to deal with fissile nuclides themselves, and refined to include later techniques for resonance absorption calculations.

The final output of the GUNYA series of computations is a 120 group set of cross sections for each nuclide used in the burnup code GYMEA (Pollard and Robinson 1966). Four separate programmes are used to cover the many intermediate calculations and data assessments which are required before satisfactory cross section representations can be achieved. The philosophy of the codes is that all experimental cross sections should be reproduced from resonance parameters alone, and that unmeasured cross sections should be estimated statistically. Such a method has the maximum amount of flexibility since variations in group boundaries or numbers of groups impose no additional difficulties.

The four programmes used in the data preparation are as follows: GUNYA 1 prepares, in a standard format, nuclear constants such as the beta decay constant and statistical resonance data. GUNYA 2 uses these constants together with all available experimental information on resonances, particularly single level resonance parameters, to prepare group cross section data. These data may be loaded directly by EDITOR (Ford 1966) to produce binary libraries used by GYMEA. GUNYA 3 and GUNYA 4 adjust the low energy data to give experimental thermal cross sections either where no resonances are available (3), or where at least one resonance has been resolved (4).

A library has been prepared using the GUNYA programmes. (Cook and Ferguson, report in preparation).

2. GUNYA 1

The GUNYA 1 programme is designed to prepare basic nuclear data for fission products in a standard library format. The basic quantities dealt with are the beta decay constants, prompt and delayed fission yields, and statistical resonance parameters. Also computed are the estimated magnitude of the effective resonance integral and the thermal cross section for each isotope.

2.1 Theory

GUNYA 1 works through the periodic table by taking twenty-one isotopes for each value of the nuclear charge and using empirical formulae to estimate various nuclear parameters. A rough estimate of the mass region for stable isotopes is selected by means of the formula of Metropolis and Reitwiesner (1950):

$$Z = A/(1.98067 + 0.0149624A^{\frac{2}{3}}) \quad , \qquad (1)$$

where Z = the nuclear charge on a stable nuclide with mass number A. The subsequent arrangement and evaluation of data can be treated in three sections.

2.1.1 Decay constants

The decay constants are read into the code where values are known accurately. Efforts are being made to estimate the values for unmeasured decay constants. However the theory of beta decay to be found in the literature (for example, Blatt and Weisskopf, 1952) cannot yet attain reliable order-of-magnitude estimates of half-lives, though for the purposes of preparing fission product data, all of the important isotope half-lives have been measured.

It may occur that an isotope which is relatively stable to beta decay undergoes neutron decay from an excited state when released as a fission product. For this reason, stable fission products must be positively identified in calculations and it is insufficient to ascertain stability from the magnitude of the beta decay constant only. Therefore, mass numbers of stable isotopes must be read into the code to ensure that the delayed fission yields are evaluated correctly. Neutron decay half-lives are known for only a small number of isotopes, but theoretical estimates are likely to be much more reliable than in the case of beta decay. Should data be required for computing transient behaviour of reactors, the option of calculating neutron half-lives can be

included in the code without difficulty. Current studies are concerned mainly with long-term burnup, so this calculation is not performed in the present version of the code. Data on beta decay constants were obtained from the O.R.N.L. Nuclear Data Sheets (1962), and England (1965).

2.1.2 Prompt and delayed fission yields

The charge dispersion of yields from fission per beta decay chain were evaluated from the experimentally verified formula of Wahl et al. (1962):

$$P(Z) = \frac{1}{\sqrt{0.9\pi}} \exp\left(-(Z-ZP)^2/0.9\right) \quad , \tag{2}$$

where $ZP = 0.424A - 2.256$, below $A = 110$,

$ZP = 0.410A - 2.901$, above $A = 110$, and

$P(Z)$ = the probability of obtaining a prompt emission of a nuclide with charge Z for a given A.

The delayed yields are read into the code, and the yields before beta emission are computed by multiplying the chain yield by $P(Z)$. The yields before prompt neutron emission are known from experiment and if some account of neutron emission is required, these experimental yields should be used. When burnup is being considered, radiochemical yields may be utilized without appreciable error being introduced.

2.1.3 Resonance data

The code evaluates the parameters of an average resonance for a given nuclide, together with the average level spacing $\overline{D}$. The basic assumption of all GUNYA codes is that the cross section for the (n,γ) reaction at temperature $0\,^{\circ}K$ is given by the super-position of many single Breit-Wigner resonances.

$$\sigma_{n\gamma}(E) = \sum_i \sum_\ell \frac{4\pi\lambda^2 \Gamma_{ni}^{\ell} \Gamma_{\gamma i}^{\ell}}{\Gamma_i^2} \frac{g_J}{1+X_i^2} \quad , \tag{3}$$

where Γ_{ni}^{ℓ} = the neutron partial width for the ℓ^{th} partial wave in resonance i.

$= \Gamma_{n\ell i} \sqrt{E}$, where $\Gamma_{n\ell i}$ is the 'reduced' neutron width, and E the neutron energy in eV,

$\Gamma_{\gamma i}$ = the radiation width for the i^{th} resonance,

$X_i = 2(E_{oi} - E)/\Gamma_i$,

E_{oi} = the resonance energy of resonance i, and

$\Gamma_i = \Gamma_{\gamma i} + \sum_l \Gamma_{ni}^{\ell}$.

The parameters used by GUNYA 1 are the averages $\overline{D}$, $\overline{\Gamma}_{n\ell}$, $\overline{\Gamma}_{\gamma}$, and the 'strength functions':

$$S_\ell = \overline{\Gamma}_{n\ell}/\overline{D} \quad . \tag{4}$$

(A) Calculation of $\overline{D}$

The present version of the code employs an empirical adaptation of the Bethe Free Gas Model (see Preston 1962). It is assumed that:

$$\log \overline{D} = f_s(A) + P(Z) + P(N) \quad , \tag{5}$$

in which:

$f_s(A)$ = a background mass-dependent function determined for the four separate cases of even-even, even-odd, odd-even, and odd-odd nuclei, and

P(Z) and P(N) are peaking functions which apply shell model corrections to the level spacing, and take account of the influence of magic numbers in Z and N that designate closed proton and neutron shells respectively.

The values of $f_s(A)$, P(Z), and P(N) are determined from the range of known nuclide level spacings, and the code uses the formula (5) to interpolate to unmeasured values of $\overline{D}$. A least squares fit of the Bethe free gas formula (Musgrove private communication) will be used in future versions of the code, to account for spin effects more adequately.

(B) Neutron widths

The reduced average neutron width for each partial wave is dealt with by assuming that the strength functions (4) are systematic functions of mass number A. This seems to be borne out by experiments (Garrison and Roos 1962). The present version of the code treats the $\ell = 0$ partial wave as well as $\ell = 1$ states. The states $\ell = 2$ become important above 1 MeV. However, fission product cross sections are so small in this region that the error in neglecting these partial waves is not serious. This is not true of fissile nuclides, nor of nuclides with large A.

The programme first calculates $\overline{D}$, then Γ_{no} from the input values of S_o.

(C) Radiation widths

The radiation widths are also taken to be systematic functions of the mass number. The available data from Hughes and Schwartz (1958) and Garrison and Roos (1962) seem to indicate that there are no appreciable shell configuration effects upon the radiation widths. Maradyan and Adamchuk (1965) have found some evidence in Nb93 that the radiation width may depend strongly upon ℓ. However, we assume that averages taken over low energy resonances are a reliable indication of Γ_γ for S states.

(D) Spin weight factors

The value of g_J in Equation 3 was taken to be unity in even-even and odd-odd nuclei and 0.5 in even-odd and odd-even nuclei. In order-of-magnitude estimates of cross sections this choice is justifiable.

(E) The energy of the lowest resonance

The energy of the lowest resonance was estimated by utilizing a formula identical to (5) for E1, with different empirical parameters. Later processing by the GUNYA codes allows this assignment to be altered to the experimental value, if determined, or to a value which yields the measured thermal cross section. Nevertheless, for nuclides where no experimental determination at all is available, this is the only technique available and must be viewed as an order-of-magnitude estimate only.

(F) Resonance integrals and thermal cross sections

The area under the resonances (3) for a 1/E flux weight is the effective resonance integral, given approximately by:

$$\text{E.R.I.} = \sum_i \frac{\pi \sigma_{oi} \Gamma_{\gamma i}}{2E_{oi}} \quad , \tag{6}$$

for infinite dilution. The programme sums all such contributions for resonances from 0.4 eV to 1 MeV and outputs this estimate as the effective resonance integral. The 1/v tail contribution is not included.

The thermal cross section at 0.025 eV is determined using Equation 3 for six positive energy resonances and six negative energy resonances. This estimate is likely to be the most unreliable output from the code, because the thermal cross section is determined chiefly by the resonance

wings of those levels closest to the origin E = 0, and these may have parameters deviating markedly from the average values, according to the Porter–Thomas distributions of partial widths (see Porter and Thomas 1956). Furthermore it depends critically upon the value of E_o assigned to the lowest energy resonance, and the assumption that the levels are equally spaced. Both of these approximations may lead to large errors.

(G) The potential scattering cross section

The potential scattering cross section is determined from the approximate formula:

$$\sigma_p = 0.33\ A^{\frac{2}{3}} \text{ barns.} \qquad (7)$$

2.2 Input

The input consists of:

(i) Three cards containing the pairs of numbers designating the range of values of Z, N, and A respectively in format (2I5).

(ii) The chemical symbols of each element arranged in ascending order of Z in format (36A2).

(iii) The peaking functions P(Z) and P(N) for the calculation of E1 and $\overline{D}$ respectively, arranged in format (7E10.3).

(iv) The values of $\Gamma_\gamma(A)$ for each mass number in format (7E10.3).

(v) The $\ell = 0$ strength functions $S_0(A)$ also in format (7E10.3).

(vi) The background terms for computing $\overline{D}$, that is $f_s(A)$, in format (7E10.3), for the cases even–even, even–odd, odd–even, and odd–odd nuclei respectively.

(vii) The background terms for computing E1 arranged in the same fashion as (vi).

(viii) An option card containing a zero, if the delayed yields are to be calculated, and unity if they are to be read in with format (I5). The option to calculate is not available nor applicable for burnup.

(ix) If yields are read in, the next set of cards contain the stable Z value for a given A, arranged in format (14I5), followed by:

(x) The delayed yields for the isotopes U233, U235, Pu239, Pu241, respectively, in format (7E10.3).

(xi) An option card containing a zero if the full range is required, unity if specific nuclides are desired, or 2 if resonance parameters only are to be calculated, followed by the number of nuclides selected, in format (2I5).

(xii) A card containing the lower and upper value of A desired, in format (2I5).

(xiii) If options 1 or 2 above are chosen, the value of Z, the chemical symbol, and the mass number of the specified nuclide, follow in format (I3,A2,I3), followed finally by:

(xiv) The beta decay constants, twenty–one values for each value of Z, arranged in format (7E10.3).

2.3 Output

The output is arranged into four standard library cards per isotope, for the library–generating option.

(i) The first card contains Z, the chemical symbol, and mass number of the isotope; the same for the product via the (n,γ) reaction; the potential scattering cross section, σ_p, the thermal cross section, the effective resonance integral, E1 and $\bar{D}$, in format:

(I3,A2,I3,2X,I3,A2,I3,2X,1P5E10.3,8H1 XS+RES).

(ii) The second card contains the Z value, symbol, and A, as above, of the isotope and its beta decay product, followed by the beta decay constant, and the four delayed yields from fission associated with the above four fissile isotopes, all in format:

(I3,A2,I3,2X,I3,A2,I3,2X,1P5E10.3,8H2 DC,YD).

(iii) The third card contains the above nuclide identification, followed by the four prompt yields, in format:

(I3,A2,I3,22X,4E10.3,8H3 YPRMPT).

(iv) Finally, there is the standard nuclear data card library statistical parameter card containing the lethargy corresponding to E1, the average spacing $\bar{D}$, the average reduced width Γ_{no}, the spin weight factor g_J, and the nuclide identification, Z, A, symbol, A, in format:

(F7.3,1PE11.3,2E10.2,10H0.0,E10.2,7H18,I3,I4,3HURP,A2,I3).

3. GUNYA 2

The programme GUNYA 2 computes group cross sections with an arbitrary set of lethargy groups for both fissile and non–fissile isotopes. In the interest of flexibility, the code will deal with elements where no resonance parameters are known, up to the case where three hundred resonances are resolved. The theory involves a combination of statistical resonance formulae with refined calculations of cross sections over the resolved region, in such a way that from one to two hundred and fifty groups may be employed without error. However, the output is specially arranged to be compatible with the input to the GYMEA burnup code (Pollard and Robinson 1966). A special version of GUNYA 2 which adjusts cross sections to compensate for approximations made in the GYMEA resonance theory has been prepared, and is available.

3.1 Theory

3.1.1 The statistical region

Let the absorption width, Γ_a, be given by

$$\Gamma_a = \Gamma_\gamma + \Gamma_f \quad . \tag{8}$$

The absorption cross section, averaged over many levels E_{oi}, can be written (U.S.A.E.C. Reactor Physics Constants 1963 (i)), from (6):

$$\langle \sigma_{abs} \rangle \approx \frac{1}{\Delta U} \int_{E_1}^{E_2} \frac{dE_o}{\bar{D}} \left(\frac{\pi \sigma_o \Gamma_a}{2E_o} \right)$$

$$= \frac{\pi \times 2.608 \times 10^6 \; g_J \; \Gamma_a}{2D \; \Delta U} \int_{E_1}^{E_2} \frac{dE_o \langle \Gamma_{n\ell} \rangle}{E_o^{\frac{3}{2}} \left(\Gamma_a + \langle \Gamma_{n\ell} \rangle \sqrt{E_o} \right)} \quad , \tag{9}$$

where D is the average level spacing and ΔU the lethargy band of integration. The brackets $\langle \rangle$ denote averaged quantities.

For states other than $\ell = 0$, the neutron reduced width is energy–dependent; therefore an approximation is made which is valid for narrow groups, namely that the energy dependent part of $\Gamma_{n\ell}$ is evaluated at the constant value of $\frac{1}{2}(E_1 + E_2)$. When the groups are very wide, the higher ℓ state contribution is insignificant, hence the approximation is justifiable in this case as well.

The integration in (9) can then be carried out to yield:

$$\langle \sigma_{abs} \rangle = \frac{8.914 \times 10^6}{\Delta U \; D} (\Gamma_{no} g_{J0} + \Gamma_{n1} g_{J1}) T_1 - (\Gamma_{no} g_{J0} T_{20} + \Gamma_{n1} g_{J1} T_{21}) \qquad (10)$$

where $$T_1 = \frac{1}{\sqrt{E_1}} - \frac{1}{\sqrt{E_2}}$$

$$T_{2\ell} = \frac{\langle \Gamma_{n\ell} \rangle}{\Gamma_a} \log \left(\sqrt{\frac{E_2}{E_1}} \cdot \frac{\Gamma_a + \langle \Gamma_{n\ell} \rangle \sqrt{E_1}}{\Gamma_a + \langle \Gamma_{n\ell} \rangle \sqrt{E_2}} \right) , \quad \text{and}$$

g_{J0}, g_J, etc. are the spin weight factors for $\ell = 0$, 1, and higher states. When dealing with fission product isotopes, it was found that only $\ell = 0$ and 1 states were required to give a reasonable representation of the cross section. When dealing with fissile isotopes, the situation is complicated by the presence of higher ℓ states and the energy dependence of the fission partial width. A special version of the code was prepared to take more detailed account of these high energy effects, and is available.

The fission and capture cross sections are obtained from (9) via the equations:

(i) $$\langle \sigma_f \rangle = \frac{\Gamma_f}{\Gamma_a} \langle \sigma_{abs} \rangle , \text{ and}$$

(ii) $$\langle \sigma_c \rangle = \frac{\Gamma_\gamma}{\Gamma_a} \langle \sigma_{abs} \rangle \qquad (11)$$

The statistically averaged scattering cross section is easily found to be given by:

$$\langle \sigma_s \rangle = \frac{1}{\Delta U} \int_{E_1}^{E_2} \frac{\pi \sigma_o \langle \Gamma_n^{\ell} \rangle}{2E_o} \frac{dE_o}{D}$$

$$\approx \frac{8.914 \times 10^6}{\Delta U \; \overline{D}} (\Gamma_{no} g_{J0} T_{20} + \Gamma_{n1} g_{J1} T_{21}) , \qquad (12)$$

where T_{20} and T_{21} are defined as in Equation 10. For a detailed account of statistical evaluation of cross sections, see Greebler and Goldman (1962)

3.1.2 The undetermined resonance region

The statistical formula (10) is valid provided there is an appreciable number of resonances per energy group. By inspection, it was found that for less than ten resonances per group, the formula begins to deviate from the direct sum of the areas given by (6); accordingly the individual contributions from equally spaced resonances are summed for such groups. Should the resolved resonance region extend directly into the statistical region, this part of the calculation is by–passed.

3.1.3 The resolved resonance region

The GYMEA oriented version of the code currently defines the resonance region as extending from 1 eV to 454 eV. In this energy range, resolved resonances require special treatment and the programme computes either 'resonance adjusted' cross sections or 'resonance removed' cross sections. Resonance adjusted cross sections compensate for the following GYMEA restrictions:

(i) The group boundaries are sufficiently spaced to allow all of the area beneath a resonance to be placed in one group, and

(ii) The neutron width and 1/E flux variation across a resonance is negligible.

The following theory replaces the previously used techniques discussed by Doherty (1963).

The cross section computed outside a resonance group is, for example:

$$\left\langle \sigma_{n,\gamma} \right\rangle = \frac{1}{\Delta U} \int_{E_1}^{E_2} \sigma_{n,\gamma}(E) \frac{dE}{E}$$

$$= \frac{1}{\Delta U} \int_{E_1}^{E_2} \sqrt{\frac{E_o}{E}} \frac{\sigma_o}{1+X^2} \frac{dE}{E}$$

$$= \frac{6.52 \times 10^5 \left\langle \Gamma_n^{\ell} \right\rangle \Gamma_\gamma g_J}{\sqrt{E_o}\, \Delta U} I \quad ,$$

where $I = 2 \left(\frac{1}{\alpha^2 \sqrt{E_1}} - \frac{1}{\alpha^2 \sqrt{E_2}} \right) + \frac{2(\alpha - \beta^2)}{4\alpha^3} \ell n \left\{ \frac{(\sqrt{E_1} + \frac{1}{2}\beta)^2 + \gamma^2}{(\sqrt{E_1} - \frac{1}{2}\beta)^2 + \gamma^2} \times \frac{(\sqrt{E_2} - \frac{1}{2}\beta)^2 + \gamma^2}{(\sqrt{E_2} + \frac{1}{2}\beta)^2 + \gamma^2} \right\}$

$$+ \frac{\beta^2 - 3\alpha}{2\gamma\alpha^3} \left[\tan^{-1} \left(\frac{\sqrt{E_2} - \frac{1}{2}\beta}{\gamma} \right) + \tan^{-1} \left(\frac{\sqrt{E_2} + \frac{1}{2}\beta}{\gamma} \right) \right.$$

$$\left. - \tan^{-1} \left(\frac{\sqrt{E_1} - \frac{1}{2}\beta}{\gamma} \right) - \tan^{-1} \left(\frac{\sqrt{E_1} + \frac{1}{2}\beta}{\gamma} \right) \right] , \qquad (13)$$

and $\alpha^2 = E_o^2 + \frac{1}{4}\Gamma^2$,

$\beta^2 = 2(E_o + \alpha)$,

$\gamma^2 = \frac{1}{2}(\alpha - E_o)$.

The contributions from all resonances are summed for each group. When resonance groups are encountered, the programme evaluates:

$$\left\langle \sigma_{ra} \right\rangle = \sum_{\text{resonances}} \left\langle \sigma_{n,\gamma} \right\rangle - \frac{\text{E.R.I.}}{\Delta U} \quad , \qquad (14)$$

where E.R.I., the effective resonance integral, is obtained from the formula (6).

As an alternative approach, used to conserve compatibility with previous techniques (Doherty 1963), the 'resonance removed' cross section may be computed instead. This version evaluates point cross sections such that the library group cross section has the value:

$$\left\langle \sigma_{n,\gamma} \right\rangle = \left(\sqrt{\frac{E_r}{E}} - 1 \right) \frac{\sigma_o \Gamma_\gamma}{\Gamma(1+X^2)} , \qquad (15)$$

for each resonance in the resonance region. Contributions from all resonances are summed, and the cross section (15) is calculated for the central energy of the group. This procedure, however, was found to be in error when a large amount of self-shielding is present.

3.1.4 The thermal region

This is defined as the energy region lying below 1 eV. Here the group boundaries are usually close together and the cross sections are calculated as point values computed directly from Equation 3. Negative energy resonances often have to be included to ensure that the resonance tails yield the correct thermal cross section at 0.0253 eV, whether or not resolved resonances have been given in the input.

In dealing with fissile nuclides, the value of $\overline{\nu}$ is assumed to be given by U.S.A.E.C. Reactor Physics Constants (1963 (ii)) as:

$$\overline{\nu} = A_f + B_f . E \quad . \tag{16}$$

3.1.5 Transport cross sections

Transport cross sections in the diffusion theory approximation are computed from the formula:

$$\sigma_{tr} = \sigma_{abs} + (1 - \overline{\mu})\, \sigma_s \quad , \tag{17}$$

where $\overline{\mu} \simeq 2/(3A)$. This approximation is valid at low energies in light nuclides, and at all energies for intermediate and heavy nuclides (Weinberg and Wigner 1958).

3.2 Input

The input consists of the following cards:

(i) One card containing the number of energy groups in format (I3).

(ii) Cards containing the group lethargy boundaries in format (12F6.2).

(iii) One card giving the number of elements to be processed, in format (I2) .

(iv) A standard resonance theory card on which is punched:

(a) the potential scattering cross section.

(b) the p-wave strength function.

(c) the p-wave spin weight factor.

(d) the constants A_f and B_f in Equation 16 to evaluate $\overline{\nu}$.

The format is (5E10.3).

(v) The standard unresolved resonance parameter card follows next. This contains the parameters of the text:

$(U, \overline{D}, \Gamma_n^o, \Gamma_\gamma, \Gamma_f, g_J, Z, A, SYMBOL, A)$

in format (F7.3,E11.3,4E10.2,4X,3H.18,I3,I4,3HURP,A2,I3), where Z is the atomic number, A the atomic mass, and SYMBOL the chemical symbol of the element.

(vi) Should resolved resonance parameters be available, these are read in, ordered in decreasing energy. The standard layout of this card is:

$(U, E_r, \Gamma_n, \Gamma_\gamma, \Gamma_f, g_J, Z, A, SYMBOL, A)$ in format

(F7.3,E11.3,4E10.2,4X,3H.17,I3,I4,3HRRP,A2,I3).

(vii) The resonance cards should end with a blank card.

3.3 Output

The standard output contains the group cross sections for the six processes

(i) (n,γ),

(ii) (n, Fission),

(iii) (n, abs),

(iv) (n, $\overline{\nu}$ Fission σ),

(v) (n, transport),

(vi) (n, 2n).

(F7.3,E11.3,4E10.2,7X,I3,3X,A2,SYMBOL,A).

The first card is a nuclide identification card on which is punched (SYMBOL,A,A,TYPE) in format (A2,I3,I3,I2). GYMEA identifies the resonance nature of the isotope by the value assigned to TYPE. If TYPE = 2, the nuclide contains resonance parameters for energies between 1 eV and 454 eV. If TYPE = 0, no resonance parameters are given and the resonance included cross sections are computed.

The title card identifying the output and library follows next.

Then come six sets of reaction cross sections arranged in format (1X,1P7E10.3), headed by title cards. The title cards identify the above cross sections.

The resolved resonance parameters, if given between 454 eV and 1 eV, follow next in standard format, arranged in descending order of energy, and headed by a comment card (* RESONANCE DATA FOLLOWS). The set of resonance parameters is concluded by a final card containing (6*0.) and then an end card, on which is punched a row of asterisks, completes the data on a given nuclide.

4. GUNYA 3

The previous code in this series, GUNYA 2, calculates, in some cases, the entire energy range of cross sections from 10 MeV to 0.001 eV, using only the statistical resonance parameters. One facet of such a computation is that the (n,γ) cross section at thermal energies should be given by the tail contribution of adjacent resonances, including negative energy levels. It is most important to reactor physics applications that this energy region of cross section should be plausibly in agreement with measured values. Where this particular calculation has to be made, the experimental information consists only of the measured cross section at 0.0253 eV, and the effective resonance integral, so that the statistical resonance parameters may have to be adjusted to agree with these two quantities.

The parameter to which the thermal cross section is most sensitive is the energy of the lowest resonance. According to its assignment, the thermal cross section may range anywhere from a low minimum value to an extremely large maximum, with perhaps four orders of magnitude separating the extremes. The purpose of this programme is to find, by an iterative process, the energy of that resonance which reproduces the measured value of the thermal cross section.

4.1 Theory

The thermal cross section is determined for the most part by the closest six positive and six negative energy resonances to the origin. The contribution from each level, assuming the levels are equally spaced, is represented by the Breit–Wigner single level formula:

$$\sigma_{n,\gamma}(0.0253\ \text{eV}) = \sum_{\text{resonances}} \sqrt{\frac{E_r}{0.0253}} \quad \frac{\Gamma_\gamma \sigma_o}{\Gamma(1+X^2)} \qquad (18)$$

where $X = \frac{2}{\Gamma}(0.0253 - E_r)$.

The known experimental thermal cross section is read in together with the statistical resonance parameters, and the code begins a search upon E_r. The first assigned value is one half a level spacing from the origin. At this value, the calculated value is approximately at the minimum. If the minimum happens to be above the measured value, the neutron width and level spacing are re–normalized until the correct result is achieved. Usually, however, the minimum lies below the measured value, so the energy of the resonance is decreased until the thermal value read in is reached. Then the revised set of resonance parameters is punched out in standard format.

4.2 Input

The input contains two cards per nuclide, and a job identification card, arranged as follows:

(i) The first card contains the number of nuclides to be processed, expressed in format (I2).

(ii) The groups of two cards per nuclide begin with the standard resonance card containing:

(a) a guess at the lethargy of the lowest resonance (which is unused),

(b) the average level spacing $\overline{D}$,

(c) the reduced neutron width Γ_n^o,

(d) the average radiation width Γ_γ,

(e) the average fission width Γ_f,

(f) the spin weight factor g_J,

(g) the charge number of the nucleus Z,

(h) the atomic mass A, and

(i) the chemical symbol of the element, SYMBOL.

These are punched as

(U,$\overline{D}$,Γ_n^o,Γ_γ,Γ_f,g_J,18,Z,A,URP, SYMBOL,A)

in format

(F7.3,E11.3,4E10.2,4X,I2,I3,I4,3HRRP,A2,I3).

(iii) The second card per nuclide is punched with the value of the measured thermal cross section in format (E10.3).

4.3 Output

(i) The first line of the printed output identifies the nuclide and its thermal cross section in format (A2,I3,13H.THERMAL X–S=,1PE10.2).

(ii) The next line gives a title 'INPUT CARD', followed by a reproduction in the printed output of the input card.

(iii) This is followed by the comparison between the input and calculated thermal values in the form:

INPUT THERMAL X–S=,1PE10.2,OUTPUT THERMAL X–S=,1PE10.2.

(iv) After the above comes the printed and punched output of the revised resonance card in the above standard format.

5. GUNYA 4

It quite often arises that the thermal cross section, determined as the residual of all the tails of experimentally resolved resonances, does not agree with the direct experimental measurement of the thermal cross section, using activation methods. The usual solution of this dilemma, with codes that deal exclusively with resonance parameters, is to fit by the least squares method to a virtual, negative energy level, whose parameters are by no means determined unambiguously. Various authors may differ widely in the results of such a fit (Stehn et al. 1965) because a wide range of possible parameters is capable of reproducing the observed "1/v" behaviour.

The simplest way to find negative energy resonance parameters, where the full extent of the thermal region is unmeasured, is to place the bound level at one average level spacing below the energy of the lowest resolved resonance, provided this energy turns out to be negative. The radiation width is usually fairly constant for a given isotope, and the average value is a plausible one to choose. Only the reduced neutron width shows violent fluctuations from resonance to resonance, so we may regard it as the main parameter to be calculated from the thermal data.

5.1 Theory

The discrepancy is defined as

$$[\sigma_{n,\gamma}]_{-} = [\sigma_{n,\gamma}]_{\text{experiment}} - [\sigma_{n,\gamma}]_{+\text{ve res.}} , \qquad (19)$$

and is the quantity to be fitted to the negative energy resonance parameters.

The code assumes that the energy of the resonance is the minimum number of average spacings D, away from the lowest energy resonance, that is required to make the resonance energy negative. Assuming an average value for Γ_γ, the equation:

$$[\sigma_{n,\gamma}]_{-} = \sqrt{\frac{E_r}{0.0253}} \; \frac{1}{\Gamma} \; \frac{\sigma_o \, \Gamma_\gamma}{(1 + X^2)} ,$$

is solved for $[\Gamma_n]_{-}$, to give:

$$[\Gamma_n]_{-} = \tfrac{1}{2}(-B - \sqrt{B^2 - 4C}) , \qquad (20)$$

where $B = \left\{ 2.0 - \frac{2.608 \times 10^6 \, g_J}{E_r \Gamma_\gamma \, [\sigma_{n,\gamma}]_{-}} \sqrt{\frac{E_r}{0.0253}} \right\}$,

$C = \Gamma_\gamma^2 + 4(E_r - 0.0253)^2$,

$\Gamma = \Gamma_\gamma + [\Gamma_n]_{-}$.

The parameters of the negative energy resonance are then punched out in standard form.

5.2 Input

(i) The first card of the input contains the number of nuclides to be processed, in format (I3).

(ii) Subsequent data are grouped in one set per nuclide, the first card being punched with the experimental cross section in format E10.3. The second card is the standard statistical resonance parameter card for the nuclide on which is punched:

(U1, $\overline{D}$, Γ_n^o, Γ_γ, Γ_f, g_J: 18, Z, A, URP, SYMBOL, A) ,

where:

U1 = the lethargy of the lowest resolved resonance,

Z = the atomic number,

A = the atomic mass, and

SYMBOL = the chemical symbol of the isotope.

The above standard format is:

(F7.3, 1PE11.3, 1P4E10.2, 4X, I2, I3, I4, 3HURP, A2, I3).

(iii) Next comes the set of resolved resonance parameter cards in any order. Each card contains the information:

(U, E_r, Γ_n, Γ_γ, Γ_f, g_J, 17, Z, A, RRP, SYMBOL, A)

where U = the lethargy corresponding to E_r, in format.

(F7.3, 1PE11.3, 1P4E10.2, 4X, I2, I3, I4, 3HRRP, A2, I3).

(iv) The end of the resonance parameter set for each nuclide should be identified with a blank card.

5.3 Output

The printed output conveys the information about the residual sum of the tails and the discrepancy, in the form:

(SUM = 1PE10.3, DISC = 1PE10.3)

This is followed by the punched and printed standard resonance parameter card showing the negative energy resonance parameters in the above standard format. The lethargy of a negative energy resonance is always put equal to zero.

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