KERNFORSCHUNGSZENTRUM

KARLSRUHE

Mai 1968 KFK 772

Institut für Neutronenphysik und Reaktortechnik

Principles of Cross Section Evaluation

J.J. Schmidt

GESELLSCHAFT FÜR KERNFORSCHUNG M.B.H.

KARLSRUHE

K E R N F O R S C H U N G S Z E N T R U M
K A R L S R U H E

Mai 1968 KFK-772

Institut für Neutronenphysik und Reaktortechnik

Principles of Cross Section Evaluation *

von

J.J. Schmidt

Gesellschaft für Kernforschung m.b.H., Karlsruhe

* Invited paper submitted to the Second Conference on Neutron Cross Sections and Technology, Washington, March 4-7, 1968

A b s t r a c t

Principles of cross section evaluation

Evaluation consists in the derivation of complete easily interpolable sets of "best" values of microscopic cross sections and parametric data from available experimental and theoretical informations in the energy range 0 to about 15 MeV and the establishment of corresponding computer nuclear data libraries for further use in reactor calculations. Gaps in the experimental information can often be filled successfully by nuclear systematics or parametrization of some nuclear theory or model like statistical reaction theory, optical or evaporation model. The main difficulty in evaluation consists in systematic discrepancies outside experimental error between different experimental data sets, which only sometimes can be resolved by renormalization. Beside the differential experimental data in some cases "clean" integral data which allow univoque conclusions to the nuclear data involved are used in the evaluation. The reliability of evaluated nuclear data sets can more and more be assessed by comparison of calculated and measured integral data e.g. from critical facilities. Generally the feedback from these "dirty" integral data to differential data is not univoque and therefore a thorough review of the basic microscopic data most probably involved preferred to a computerised data adjustment that may be physically incorrect.

The field of evaluation of neutron cross sections has its origin in the reactor theory. As is well known the reactor theory deals with the solution of the Boltzmann neutron transport equation and of equations derived from it in various approximations in order to describe the neutron physical behaviour of nuclear reactors including safety coefficients like the Doppler coefficient. In these equations neutron cross sections enter as continuous functions of neutron energy and angle and other energy dependent data like fission spectra and numbers of prompt fission neutrons, resolved and statistical resonance parameters. As the modern computer capabilities allow and force increasing refinements of the reactor theory methods which have to be considered in parallel with steady refinements of the reactor physics measurement techniques, more and more detailed and reliable values have to be prepared for these nuclear data.

Every evaluation of neutron nuclear data for a given element or isotope today has therefore to fulfill the following general requirements. Reactor neutrons cover energies between about 0 and 15 MeV. In this energy range no reaction, the neutrons can undergo from physical grounds, can be left out in an evaluation. Furthermore, as the reactor physicists are interested in the detailed description of thermal as well as intermediate and fast reactors, an evaluation has to consider the subranges of thermal, resonance and fast neutrons in corresponding similar detail. Therefore, the density of the energy and angular mesh points, at which the nuclear data have to be evaluated, has to be as great as to describe the functional dependence of the data in a physically satisfactory almost monochromatic way so as to allow an as simple as possible interpolation between neighbouring data points. Linear interpolations on log-log, log-linear or linear-linear scales are most frequently used. In the regions of isolated narrow resonances, where in a double-linear interpolation scheme thousands of data points would be needed for a satisfactory representation of the cross sections, a parabolic interpolation appears to be more appropriate and helps to spare computer storage. Perhaps in the computers of the third generation with their very large storage capacities this restriction can be omitted and the double linear interpolation scheme be adopted throughout. In those special cases in which a cross section or a distribution can be parameterized in a simple and univoque way as e.g. in the case of a pure one level Breit-Wigner cross section, it could suffice to evaluate and store only the parameters. For checking purposes, however, it is advisable to store not only the parameters, but also the data points: group constants for example should come out the same, whether they are calculated from parameters or from data points. According to the different

cross section behaviour, particularly in the thermal and resonance regions, the energy subdivision will obviously be different for each element or isotope.

In order to fulfill these requirements the evaluation physicist has to consider all available sources of information, to assess critically their reliability and value and to derive, by selection, averaging, inter- or extrapolation or other relevant methods, from the available informations a univoque set of so-called "best" data. The informations which are used in evaluation come from nuclear data measurements, nuclear theories or models and from nuclear systematics. The main basis is the experimental information like measurements of cross sections as a function of the neutron energy, of angular or energy distributions in elastic or inelastic neutron scattering and theoretical interpretations of measurements like the derivation of resonance parameters from measured resonance cross sections, or the interpretation of measured inelastic scattering distribution in terms of nuclear temperatures. In the case of gaps or discrepancies in this basic information recourse must be held to some nuclear theory or model or nuclear systematics considerations. In the following we shall briefly discuss the principal methods used in the evaluation of neutron cross sections and parametric data in the ranges of thermal, resonance and fast neutrons. For simplicity we shall confine our discussion to medium weight and heavy nuclei.

The thermal energy range, with the exception of the rather complex thermal scattering laws, which we omit from our considerations, presents only minor difficulties in evaluation. To begin with medium weight and nonfissionable heavy nuclei, generally pointwise σ_T data and σ_γ values as averages over thermal reactor spectra mostly reduced to thermal energy (0.025 eV, the most probable neutron energy in a pure Maxwellian neutron spectrum at room temperature) are available from experiment. The remaining data are easily derived in the following way. In many cases the capture cross section in the thermal range follows a pure 1/v-law. This 1/v-law valid for positive as well as negative energy resonances is easily derived from resonance theory under the conditions that the resonance energies E_r are sufficiently far apart from the thermal range, that the resonance half widths are small compared to E_r, and that many exit channels are available in resonance capture, which lead to a cancelling of interference terms between different capture resonances and channels. The proportionality constant in the 1/v-law is fixed by the "best" value of the capture cross section at thermal energy which can be obtained by weighted averaging of the individual experimental

values. If the above first two conditions for a 1/v-law are not fulfilled, but still the third one, which is certainly the case for non-magic nuclei, i.e. if the resonances come close to thermal energies, then the cross section in the thermal range can be calculated from one level Breit-Wigner contributions of all known positive s-wave resonances (the contributions of higher l-wave resonances tend to zero for decreasing neutron energy) and of one assumed negative resonance. The neutron width and the position of the negative resonance can be fixed by fitting the cross section contributions of the negative resonance to the best values of the thermal total and capture cross sections. The capture width of the negative resonance can generally be chosen as equal to the average value obtained from the measured Γ_γ of the positive energy resonances, which according to the third condition above obey rather narrow distributions. Best values of $\sigma_T(E)$ are obtained by simple averaging of the experimental values and $\sigma_n(E)$ as the difference $\sigma_T(E) - \sigma_\gamma(E)$.

For the most important <u>fissionable nuclei</u> generally pointwise and thermal experimental values for σ_T, σ_f, α (or η) and occasionally pointwise σ_n values are available, from which one has to construct an internally consistent set of "best" cross sections as a function of the neutron energy. Obviously, the evaluation procedure to be chosen depends on the available data types. Most commonly $\sigma_T(E)$ and $\sigma_f(E)$ can be fixed by averaging experimental data, $\sigma_n(E)$ be derived from experimental data or from resonance theory, $\sigma_\gamma(E)$ be obtained by subtraction and $\alpha(E)$ as the ratio $\sigma_\gamma(E)/\sigma_f(E)$. The quantity η important for the determination of the fuel conversion capability of a reactor can then be calculated from α and best values of $\bar{\nu}$ which in turn can be derived from direct measurements at thermal energies. According to the most accurate available measurement due to Bollinger et al. [1] on $\bar{\nu}(E)$ of Pu^{239} at thermal and epithermal energies, $\bar{\nu}$ is constant in this region and equal to the thermal value within experimental limits which are almost comparable with the best precisions of about 1% attainable in modern $\bar{\nu}$ measurements. Thus, $\bar{\nu}$ may safely be taken as constant in the thermal and resonance energy ranges. Typical examples of evaluations of "best" thermal cross section values are the works of Westcott et al. [2] and of Sher and Felberbaum [3], for evaluations of "best energy dependent cross sections in the thermal range we refer e.g. to the works of Barrington et al. [4] and Joanou and Drake [5] as typical examples.

The evaluation of cross sections in the resonance range of neutron energies generally presents much greater difficulties, particularly for fissionable nuclei. Typically transmission and partial cross section measurements of varying energy resolution are available which subdivide the resonance range in two parts one in which almost all of the neutron resonances are resolved and an other one at higher energies in which the experimental overlapping of the resonances, due to the finite energy resolution and/or to the increasing importance of higher l-wave resonances, does no more allow the interpretation of the measured cross sections in terms of individual resonances. Because the experimental energy resolution is never exactly monochromatic, the true physical limit between resolvable and overlapping resonances is higher than that attainable by experiment. In typical presently available high resolution transmission measurements resonances can be resolved in medium-weight nuclei up to several 100 keV [6,7], in heavy non-fissionable nuclei to several keV [8,9], in fissionable nuclei to a few 100 eV [10,11]. Generally partial cross section measurements are more difficult and show worse resolution than transmission measurements. Thus, resonance neutron widths derived from transmission measurements are generally known to higher neutron energies than partial reaction widths. The measured resolved resonance cross sections are almost exclusively and successfully interpreted in terms of various approximations to the general R-matrix theory of resonance reactions [12] developed in the past. In the overlapping resonance range only a parameterisation of measured cross sections over groups of resonances is possible and concerning the energy dependence of the cross sections one has to rely on fluctuating, often discrepant experimental results or on statistical theory estimates from average resonance parameters and statistical distributions. We consider these points in more detail below.

In medium-weight nuclei at present the experimentally resolvable resonance range generally ends below the lowest inelastic scattering threshold. The total cross section is almost equal to the scattering cross section, the capture cross section being only a small component. Thus, the σ_T measurement can be described by the R-matrix theory simplified to only one open channel, i.e. the elastic scattering channel, with various subchannels according to different allowed combinations of neutron orbital and resonance total angular momenta [6,13,14]. In addition σ_γ measurements are available, which generally reveal more higher l-wave resonances for which Γ_γ is larger than Γ_n. These can generally be interpreted by superposition of single level Breit-Wigner terms.

An evaluation of the nuclear data must specify the resonance parameters including total and partial widths and resonance spins and the energy dependence of σ_T, σ_γ and σ_n. As far as possible resonance parameter and cross section "best" values should be mutually consistent. The σ_T measurements generally agree within experimental error, except mainly for differences introduced by different energy resolutions; for example a better resolved measurement might reveal more resonances than a worse resolved one. The σ_γ measurements, however, often show great differences in resolution and large systematic discrepancies which in the simplest cases are due to wrong normalisation or impurity admixtures in the samples; as a typical example we discussed recently various discrepant σ_γ measurements in the keV range on Fe [15]. Now most commonly neutron widths corresponding to the analysis of the best resolved σ_T measurement or weighted averages of neutron widths from different about equally well resolved σ_T measurements are taken as "best" values and the natural line shape of the scattering cross section is recalculated from these neutron widths. In the case of several measurements this simple procedure obviously is only allowed, if the analysis of all these measurements has been done with the same and correct theory. This is not always the case. To give an example transmission measurement on medium weight nuclei in the past have often been interpreted by the so-called Bethe formula [16] (see e.g. references [17] and discussion in reference [14], section III 1) for which the scattering matrix is not unitary and, which is inadequate to describe the often observed complex interference between different scattering resonances as does the correct one channel multilevel formula.

In such a case a reanalysis of the measurement concerned in terms of the correct theoretical description has to be done, before it can be combined with other analyses to "best" data. The difficulties in the evaluation of Γ_n and $\sigma_n(E)$ are generally small compared to those encountered in the evaluation of Γ_γ and $\sigma_\gamma(E)$. In most cases one can not simply average the existing σ_γ measurements, because the discrepancies due to systematic errors can only rarely be removed. Then one has essentially to select one experimental data set by a critical judgement of the different experiments or by nuclear systematics considerations or just by physical imagination and to take over the Γ_γ corresponding to this data set from the experimental analysis or to do oneself this analysis. Then one can calculate $\sigma_\gamma(E)$ in the natural line shape from these Γ_γ and the Γ_n from the transmission measurements. For those higher resonances, for which only the Γ_n are available and, for which the σ_γ measurements do no more allow a resonance analysis in terms of Γ_γ,

the average of the known Γ_γ for the lower resonances can be taken. In many cases up to recent days the σ_γ measurements were even too crude as to allow an interpretation in terms of resonance Γ_γ. In those cases assuming an infinitely large number of exit channels in capture, thus constant Γ_γ from resonance to resonance, one could choose measured values of the non-1/v capture resonance integral or of the capture cross section at thermal energy recalculated from resolved resonance contributions or interpolations between known $\bar{\Gamma}_\gamma$ of neighbouring nuclei using the fact of the rather smooth A-dependence of Γ_γ in order to get an estimate of $\bar{\Gamma}_\gamma$ for a given isotope. As an example we derived $\bar{\Gamma}_\gamma$ for the main Ni isotopes from known isotopic thermal σ_γ values and calculated $\sigma_\gamma(E)$ from these $\bar{\Gamma}_\gamma$ and known Γ_n values up to a few 100 keV (|14|, section III 4). We leave aside here additional difficulties introduced by the problems of isotopic and spin identification of resonances in elements consisting of several similarly important isotopes.

Heavy nonfissionable nuclei like Th^{232} or U^{238} represent up to a few keV, where p-wave resonances become increasingly important, excellent examples of almost pure s-wave one level Breit-Wigner cross section shapes with very few exceptions in which small distances between neighbouring large resonances occur. At epithermal energies, due to the average increase of Γ_n with $\sqrt{E}$ and the constancy of Γ_γ, the capture process dominates, whereas with increasing neutron energy the elastic scattering becomes more and more prominent. Mostly σ_T measurements for various sample thicknesses, allowing an interpretation of the resonances in terms of Γ_n and Γ_γ, and also some σ_γ measurements, which together with the σ_T measurements allow a direct determination of Γ_γ, are available. The fact that the resonances are so narrow and far apart explains the rather good agreement in the resonance parameters derived from earlier worse resolved and modern high resolution measurements. Thus, best values of resonance parameters are mostly easily obtained (sometimes after rejection of statistical scatter erroneously interpreted as resonances) by weighted averaging of the individual experimental results. Generally Γ_n are determined to much higher energies than Γ_γ. As the measured Γ_γ correspond to the theoretically expected narrow distributions it is justified to assume the average of the known Γ_γ for those resonances for which Γ_γ is not known. Then $\sigma_n(E)$ and $\sigma_\gamma(E)$ can be calculated from a superposition of single level Breit-Wigner terms which are the same formulae generally used in the interpretation of the measured cross sections for these nuclei. Only in the vicinity of broad, closely lying resonances level-level interference needs to be taken into account in the scattering cross section. All other cross sections follow by wellknown formulae from these two.

The evaluation of consistent resonance parameter sets and cross sections for fissionable nuclei represents one of the most difficult, but simultaneously physically most interesting problems in the evaluation field. This is particularly due to the very complex resonance structure, particularly of σ_f, to the generally very small level distance partly due to the superposition of two s-wave level sequences, to difficulties of spin assignment to resonances of these nuclei like U^{235} with high ground state spin and not very different g-factors. For the main fissionable isotopes many measurement series are available particularly for σ_T and σ_f and more recently also for η, α or σ_γ and for σ_n. However, unfortunately neither these measurements nor the resonance parameter sets derived from these measurements are generally in the desirable agreement. The reasons for these discrepancies are manyfold: different normalisation (e.g. in σ_f measurements), different energy scale, different energy resolution, different statistical accuracy, unsufficiently corrected background effects etc.; they reflect the great experimental difficulties involved particularly in the partial cross section measurements on fissionable nuclei. Furthermore only very few of the available measurement series yield enough information for the derivation of a complete set of widths and quantum numbers of a given resonance. Finally a whole series of different shape and area resonance analysis methods and various approximations to the many-channel R-matrix theory, ranging from the still most frequently used simple one level formula over the many capture, few fission channel approximations due to Vogt [18] and to Reich and Moore [19,20] to the most sophisticated many-level analyses of Adler and Adler [21].

Because of these differences and discrepancies an evaluation, in a strict sense, would have to go back to the original data, try to understand as much of these discrepancies, to reconcile as far as possible different measurements of the same quantity , select the measurements according to their quality in statistical scatter, resolution etc., to analyse the selected data sets in terms of one and the same appropriate approximations to the R-matrix theory (taking into account the different Doppler and energy resolution broadening of the resonances in different measurements), to derive "best" resonance parameters, and finally to recalculate partial and total cross sections in natural line shape with the same formulae from the "best" parameters. The excellent work of Adler and Adler [21] on U^{235} resonances shows how much labour is involved in such a thorough evaluation.

Most of the existing evaluations are based on less sophisticated and laborious methods. They use the fact that the one level interpretation yields resonance half widths not very different from the multilevel results, that most of the experimental resonance analyses use the one level formula and that (particularly with the exception of U^{233} and Pu^{241} resonances) the main part of the resonance fission cross section in the vicinity of the resonance peaks (except in the dips between the resonances, where interference effects become important) can be rather satisfactorily described by the one level formula. Several simple methods, based on extensive applications of the one level formula, for the derivation of complete parameter sets for a given resonance from various carefully preselected experimental sources are discussed in reference [14], sections IV 1 and IV 3. We consider only one typical example. Given an isolated resonance and the following experimental information: η in the resonance peak represented by

$$(1) \qquad \eta \approx \bar{\nu} \frac{\sigma_{of}}{\sigma_{o\gamma} + \sigma_{of}} = \bar{\nu} \frac{\Gamma_f}{\Gamma_\gamma + \Gamma_f} = \bar{\nu} \frac{\Gamma_f}{\Gamma - \Gamma_n}$$

(σ_{of}, $\sigma_{o\gamma}$ = peak fission and capture cross sections of the resonance considered), furthermore the quantities $\sigma_{of} \cdot \Gamma$, σ_{of} and Γ from a combined area and shape analysis of measured σ_f values. Considering that in the one level approximation

$$(2) \qquad \sigma_{of}\Gamma = \sigma_o \Gamma_f = 4\pi \lambda^2 (E_o) \frac{g_J \Gamma_n \cdot \Gamma_f}{\Gamma}$$

(E_o = resonance energy, λ = reduced neutron wave length, g_J = statistical weight factor) and inserting Γ_f from equation (1) one gets for Γ_n the following quadratic equation

$$(3) \qquad \Gamma_n \left(1 - \frac{\Gamma_n}{\Gamma}\right) = \Gamma'_n = \frac{(\sigma_o \Gamma_f) \cdot \bar{\nu}}{2\pi \lambda^2 (E_o)}$$

Here we have refused to a determination of the resonance spin and have set $g_J = 1/2$. Equation (3) is easily solved to give

$$(3a) \qquad \Gamma_n = \frac{1}{2} \Gamma \left\{1 - \sqrt{1 - 4 \frac{\Gamma'_n}{\Gamma}}\right\}$$

Γ_f then follows from equation (1) and Γ_γ from the difference $\Gamma - \Gamma_n - \Gamma_f$.

Having established in this way complete one level parameter sets for the available resolved resonances, one can now calculate partial and total cross section, α and η "best" values with the same one level formulae in natural line shape.

We next consider briefly the region of overlapping resonances. In medium weight nuclei "best" σ_T values are usually obtained from the best resolved measurements available which follow most closely the true physical fluctuations of the cross section. For σ_γ some sophisticated average through generally differing experimental data has to be chosen. Also inelastic scattering to the lowest excited levels sets in; we deal with the inelastic scattering further below. σ_n is usually obtained by subtraction of the sum of the other partial cross sections from σ_T. For the calculation of energetic self shielding factors for the overlapping resonances average (elastic and inelastic) neutron and capture widths, (elastic and inelastic) strength functions and average level spacings for different (l,J)-combinations and as functions of the neutron energy must be made available. Here the simplest possible way is to take Γ_γ independent from l, J and E, to adapt appropriate optical potentials to a "best" description of an average through the experimental σ_T values and of measured elastic scattering angular distributions in order to derive the strength functions and to use the appropriately parameterised Fermi gas model for the prediction of the energy and spin dependences of the average level spacing; the average scattering widths are then obtained from strength functions and average level spacings.

In heavy non-fissionable nuclei the overlapping resonance range, in which cross section fluctuations outside statistical error can be observed, covers s and p-wave neutrons. The cross sections in this range are either directly taken from experiment or calculated from average s and p-wave resonance parameters and statistical distributions. Generally a statistical theory obtained from averaging single level Breit-Wigner terms is sufficient and average interference terms can usually be neglected as far as the condition $\bar{\Gamma}/\bar{D} < 1$ is not hurted ([14], section II 2). The understanding of the usual discrepancies between different σ_γ measurements again represents the main problem here. Average s-wave resonance parameters ($\bar{\Gamma}_n$, $\bar{\Gamma}_\gamma$, $\bar{D}$) are generally directly derived from the parameters of the resolved resonances, the p-wave strength function follows from fits of statistical theory expressions to averaged experimental σ_T values in the keV range. The energy dependence of $\bar{\Gamma}_n$ is specified by the well known centrifugal barrier penetration factors, the energy and resonance spin dependences of $\bar{D}$ again by

an appropriate Fermi gas model. The parity dependence of $\bar{D}$ has been shown by Ericson [22] to be very small and is usually neglected. Commonly $\bar{\Gamma}_\gamma$ is assumed to be independent of l and J; for U^{238} the equality of s and p-wave capture widths appears to be confirmed within experimental accuracy by the p-wave resonance measurements of Thomas and Bollinger [23]. The level spacings for each individual resonance sequence are assumed to obey a Wigner distribution, the reduced neutron widths a Porter-Thomas distribution, assumptions which are well verified by the existing experiments (see e.g. [24]). For nuclei with a ground state spin I=0 it happens that for certain $\ell>0$ resonance series the same resonance J value is reached by combinations of l with the two different channel spins $j_\pm = I \pm 1/2$. Under the probably justified assumptions that possible interactions between nuclear and neutron spins are small and can be neglected and, that no correlations exist between Γ^J_{nj+} and Γ^J_{nj-}, the reduced neutron widths

$$\Gamma_n^{(o)lJ} = \sum_{j=-1/2}^{+1/2} \Gamma_{nj}^{(o)lJ}$$

of such (l,J) resonance series obey a χ^2 distribution with two degrees of freedom (see e.g. [25]). Interpretation of evaluated resonance capture widths in terms of χ^2 distributions generally yields large numbers of exit channels typically ranging from 20 to 40 corresponding to rather narrow distributions; therefore in the calculations one uses almost exclusively constant capture widths in accord with a δ-function distribution. The same parameters from which the average energy dependence of the cross sections is calculated, serve in the calculation of Doppler coefficients and of temperature dependent energetic self shielding factors in the unresolved resonance range.

Whereas for <u>fissionable nuclei</u> almost all what has been said for non-fissionable nuclei remains true, a large additional difficulty is introduced by the fission component. We need only to remember the recent measurements [26-28] strongly deviating from former experiments and the discussions still not completed concerning the energy dependence of α and of σ_f for Pu^{239} in the higher eV and lower keV energy range [26,28] in order to demonstrate the difficulties in evaluating "true" $\sigma_f(E)$ and $\alpha(E)$ values in the unresolved resonance range. For estimates of $\bar{\Gamma}_f^{lJ}(E)$ (l=0,1) several ways are possible. Usually one either relies completely on the well known channel theory formula

$$(4) \qquad \frac{2\pi\,\bar{\Gamma}_f^{J\pi}(E)}{\bar{D}^{J\pi}(E)} = \sum_i \frac{1}{1+\exp\left\{2\pi\,\frac{E_i^{J\pi}-E}{\hbar\omega_i^{J\pi}}\right\}}$$

($E_i^{J\pi}$, $\hbar\omega_i^{J\pi}$ = position and width of the i-th saddle point state belonging to the same J,π) valid for saddle point shapes of inverted harmonic oscillators and has then to specify barrier positions and widths from saddle point state systematics [29,30] and/or fission threshold experiments [31,32]. Or one uses this procedure only for p-wave neutrons and takes equation (4) for s-wave neutrons with a most probable spin independent barrier width of about 500 keV (see e.g. [31]) and fixing the saddle point positions by the $\bar{\Gamma}_f$ values calculated from the resolved resonance Γ_f. Also "best" values of $\alpha(E)$ can be used in order to fix $\bar{\Gamma}_f(E)$ with or without specification of the spin dependence ([14], sections IV 1 and IV 3, |33|). Finally combinations of these procedures are possible. In every case, however, one has to assure that on the average statistical theory cross section estimates from the average resonance parameters are or become consistent with the cross section "best" values derived from the experimental data.

Evaluation principles and methods in the <u>fast neutron energy range</u> are generally not as difficult and are well known. So we can be rather brief here. Neutron interactions in <u>medium weight nuclei</u> in addition to those already described before are inelastic scattering and absorption processes like (n,p) and (n,α). The inelastic scattering range is subdivided into two subranges. The lower goes from the lowest threshold generally to several MeV, where either measurements of individual level excitation cross sections are available or, where positions, spins and parities of the rest nucleus levels are known and enable rather reliable theoretical predictions of inelastic excitation cross sections by the theory of Hauser and Feshbach [33] with inclusion of the so-called statistical fluctuation factors.

In the higher subrange above several MeV inelastic scattering to individual levels can not more be specified experimentally. Only broad energy distributions from inelastic scattering can be measured and interpreted or predicted by an evaporation model. Recent theoretical refinements of the level density expressions and parameters [34] particularly allow more sophisticated interpretations and predictions of "continuous" inelastic scattering spectra than the older evaporation formulae (see e.g. [35]). In the evaluation of the experimental

data for $\sigma_{n'}^{exc}$ one has to pay particular attention to the fact whether the measurements have been corrected for multiple scattering and for neutron attenuation in the sample in order to get no overestimates; we refer here for example to an extensive discussion of available $\sigma_{n'}^{exc}$ measurements on Fe in reference [14], section V 3. The total σ_n in the "continuum" range are generally not directly measured and have therefore to be derived from the difference $\sigma_X - \sigma_p - \sigma_\alpha - \sigma_{2n} - \sigma_\gamma - \ldots$ As to $\sigma_p(E)$ and $\sigma_\alpha(E)$ one has still to rely as far as possible on experimental data which, however, are often discrepant e.g. by different normalization; the statistical theory for these processes, in spite of the progress made (see e.g. [36]), is apparently still not able to describe measured cross sections within experimental accuracy and thus to make reliable predictions of unknown cross sections (see reference [14], section V). σ_n is generally derived as the difference $\sigma_T - \sigma_X$.

Unfortunately the quality and energy resolution of the available measurements for different processes are quite different. In a typical example σ_T might still show physically real fluctuations outside statistical scatter, where for a partial cross section or σ_X at worst only a few broadly resolved points are available. This inconsistency between different experimental data sets is also reflected by evaluated data sets; it leads particularly to "local" errors in those data like σ_n which are obtained by subtraction and not from direct experimental information. Unfortunately the refolding of an experimental data set of bad resolution to the good resolution of a transmission measurement is generally either not possible or at least not univoque.

For heavy fertile and fissionable nuclei one has in addition to do particularly with $\sigma_f(E)$ and $\bar{\nu}(E)$. For fast energies there is generally much better agreement between different σ_f measurements than in the keV range. The evaluation of $\bar{\nu}(E)$ for a nuclide presupposes the derivation of basic $\bar{\nu}$ standards from the available experimental data and the renormalization of the experimental $\bar{\nu}$ values to these standards. Concerning the gross structure the available experimental information appears to indicate that the energy dependence of $\bar{\nu}$ can be represented over the whole energy range by a simple second or third order polynomial in E or by piecewise linear approximations, the free parameters being fixed by a least squares adaptation to the experimental data. However, by this procedure possible fine structures in $\bar{\nu}(E)$ like those observed by Blyumkina et al. [37] on U^{235} in the several 100 keV range (but not confirmed by other authors, see [14], section VI 1g) and attributed to fission channel effects get lost.

Elastic scattering angular distributions in medium weight and heavy nuclei are generally isotropic in the centre-of-mass system up to energies of the order of 10 keV where s-wave scattering is predominant. In the resonance range in medium weight nuclei composed of resonances with different l and J values the experimental information on $\sigma_n(E,\vartheta)$ is still not detailed enough and "best" values of $\sigma_n(E,\Theta)$ have to be evaluated from a rather restricted number of measured distributions. In heavy nuclei with the much larger level density, $\sigma_n(\Theta)$, within the experimentally possible resolutions, is already in the keV range a rather smooth function of the neutron energy. In the MeV range, as is well known, the optical model with appropriate parameterisation is able to reproduce the few available $\sigma_n(\Theta)$ measurements about within experimental accuracy and can thus be used rather reliably for interpolations and predictions of $\sigma_n(\Theta)$.

From the available integral data generally only those rather few which might be called "clean" can directly be used in the evaluation of "best" microscopic data. By "clean" integral data we mean those in which no spatial dependence enters and, in which, directly in the experiment and/or afterwards by corrections, the neutron energy spectrum is completely and univoquely specified as a simple function of the neutron energy and, from which one can draw univoque conclusions to certain microscopic nuclear data. Typical quantities are the infinite dilute non-1/v capture or activation resonance integral already mentioned above, which can be used for the estimate of an average capture width, or measurements of average (n,p) or (n,α) cross sections in a fission spectrum, which can be used for renormalization of $\sigma_p(E)$ or $\sigma_\alpha(E)$ data.

The reliability of evaluated nuclear data sets can more and more be tested by comparison of calculations, in which these data are used converted to groups constant sets, and measurements of integral data like spectral indices, prompt neutron decay constants, fission and capture rate traverses, breeding ratios and others in critical facilities [38,39]. Particularly the effect of new measurements of important cross sections, whose results deviate from the respective evaluated "best" data [44], on the prediction of integral measurements is studied with "interim" group cross section sets which differ from the respective "best" sets only in these new data and yield a test of the reliability of these measurements [39]. The results of those integral comparisons and tests give indications as to which microscopic "best" data might be in error and would have to be reinvestigated. Several computer programs have recently been developed [40-43] which allow an adjustment of group constants by

fits to sets of measured integral data. However, the feedback from those integral data as were mentioned before to differential data or even only to group constants is generally not unequivocal ; the adjustment may even lead to physically wronger results. This has the consequence that different adjusted data sets are likely to fit a series of critical facility measurements equally well. Furthermore one can not be sure that such a group cross section set adjusted for critical facility data will allow more correct predictions of the physical properties of large power reactors. Therefore, in order to get better approximations to the physically true cross section shape which, on the nuclear data side of the problem, alone can guarantee throughout correct reactor physics calculations, we would prefer a thorough reevaluation of the basic microscopic data to a computerized group cross section adjustment.

Literature references

1. L.M. Bollinger, R.E. Coté, G.E. Thomas, Geneva Conf. 1958, P/687; Proceed. Vol 15, p. 127.

2. C.H. Westcott, K. Ekberg, G.C. Hanna, N.J. Pattenden, S. Sanatani, P.M. Attree, IAEA Atomic Energy Review 3, 1, 1965.

3. R. Sher, J. Felberbaum, BNL-918 (EANDC(US)-75"U"), 1965.

4. E.P. Barrington, A.L. Pope, J.S. Story, AEEW-R-351, 1964.

5. G.D. Jcanou, M.K. Drake, GA-5944 (NASA CR-54263), 1964.

6. C.D. Bowman, E.G. Bilpuch, H.W. Newson, Ann. Phys. (N.Y.) 14, 319, 1962

7. S. Cierjacks, P. Forti, D. Kopsch, L. Kropp, H. Unseld. IAEA Conf. on Nucl. Data for Reactors, Paris, October 1966, Proceed. Vol. I, p. 444; S. Cierjacks, Ph.D. thesis, unpublished.

8. J.B. Garg, J. Rainwater, J.S. Petersen, W.W. Havens, Jr, Phys. Rev. 134 B, 985, 1964.

9. W. Kolar, K.H. Böckhoff, EANDC(E)-86"AL", 1967.

10. A. Michaudon, H.Derrien, P. Ribon, M. Sanche, Nucl. Phys. 69, 545, 1965.

11. C.A. Uttley, EANDC(UK)-40"L", 1964.

12. A.M. Lange, R.G. Thomas, Rev. Mod. Phys. 30, 257, 1958.

13. G. Rohr, Nucl. Phys. A104, 1 , 1967.

14. J.J. Schmidt, KFK-120 (EANDC(E)-35"U"), part I, 1966.

15. J.J. Schmidt, IAEA Conf. on Nuclear Data for Reactors, Paris, October 1966, Proceed. Vol. II, p. 279.

16. H.A. Bethe, Rev. Mod. Phys. 9, 69, 1937; H.A. Bethe, G. Placzeck, Phys. Rev. 51, 450, 1937.

17. C.T. Hibdon, Phys. Rev. 118, 514, 1960; Phys. Rev. 122, 1235, 1961; Phys. Rev. 124, 500, 1961.

18. E. Vogt, Phys. Rev. 112, 203, 1958; Phys. Rev. 118, 724, 1960.

19. C.W. Reich, M.S. Moore, Phys. Rev. 111, 929, 1958.

20. M.S. Moore, C.W. Reich, Phys. Rev. 118, 718, 1960.

21. D.B. Adler, F.T. Adler, ANL-6792, 695, 1963.
Conf. on Neutron Cross Section Technology, Washington, March 1966, Proceed. Vol. 2, p. 873; final report Subcontract AEC-BNL-006977, 1966.

22. T. Ericson, Advances in Phys. 9, 444, 1960.

23. G.E. Thomas, L.M. Bollinger, EANDC Conf. on the Study of Nucl. Structure with Neutrons, Antwerp. 1965, P/96.

24. J.J. Schmidt, ANS National Topical Meeting on Reactor Physics in the Resonance and Thermal Regions, San Diego, February 1966, Proceed. Vol. II, p. 223.

25. C.E. Porter, R.G. Thomas, Phys. Rev. 104, 483, 1956.

26. P.H. White, J.G. Hodgkinson, G.J. Wall, J. Nucl. En., Pts. A/B, Reactor Sci. Techn. 19, 325, 1965.

27. M.G. Schomberg, M.G. Sowerby, F.W. Evans, IAEA Sympos. on Fast Reactor Physics and Related Safety Problems, Karlsruhe, November 1966, Paper SM-101/41.

28. W.B. Gilboy, G.F. Knoll, IAEA Conf. on Nucl. Data for Reactors, Paris, October, 1966, Proceed. Vol. I, p. 295.

29. J.E. Lynn, IAEA Conf. on Nucl. Data for Reactors, Paris, October 1966, Proceed. Vol. II, p. 89.

30. J.J. Griffin, IAEA Seminar on the Physics and Chemistry of Fission, Salzburg, March 1965, Proceed. Vol. I, p. 23.

31. J.A. Northrop, R.H. Stokes, K. Boyer, Phys. Rev. 115, 1277, 1959.

32. H.C. Britt, F. Plasil, Phys. Rev. 144, 1046, 1966.

33. W. Hauser, H. Feshbach, Phys, Rev. 87, 366, 1952.

34. A. Gilbert, A.G.W. Cameron, Can. J. Phys. 43, 1446, 1965.

35. J.M. Blatt, V.F. Weißkopf, Theoretical Nuclear Physics, J. Wiley and Sons, New York, 1952, chapter VIII.

36. H. Büttner, A. Lindner, H. Meldner, Nucl. Phys. 63, 615, 1965.

37. Y.A. Blyumkina et al., At. Energ. 15, 64, 1963; translated in Sov. J. At. En. 15, 725, 1964; Nucl. Phys. 52, 648, 1964.

38. D. Stegemann et al., IAEA Sympos. on Fast Reactor Physics and Related Safety Problems, Karlsruhe, November 1967, paper SM-101/8 (KFK 626, EUR 3670e).

39. H. Küsters et al., IAEA Sympos. on Fast Reactor Physics and Related Safety Problems, Karlsruhe, November 1967, paper SM-101/12 (KFK 628, EUR 3672e)

40. P.C.E. Hemment, E.D.Pendlebury, Int. Conf. on Fast Critical Experiments and their analysis, Argonne, October 1966, ANL-7320, p. 88.

41. A. Pazy, G. Rakavy, Y. Reiss, Y. Yeivin, IAEA Conf. on Nucl. Data for Reactors , Paris, October 1966, Proceed. Vol. II, p. 309.

42. G. Rakavy, Y. Reiss, D. Samoucha, Y. Yeivin, IAEA Sympos. on Fast Reactor Physics and Related Safety Problems, Karlsruhe, November 1967, paper SM-101/41.

43. L.N. Usachev, S.M. Zaritsky, IAEA Conf. on Nucl. Data for Reactors, Paris, October 1966, Proceed. Vol. II, p. 321.

44. W.P. Pönitz, D. Kompe, H.O. Menlove, K.H. Beckurts, IAEA Sympos. on Fast Reactor Physics and Related Safety Problems, Karlsruhe, November 1967, paper SM-101/9 (KFK 635, EUR 3679e).