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INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA CONSULTANTS MEETING
ON
THE USE OF NUCLEAR THEORY IN NEUTRON NUCLEAR DATA EVALUATION

International Centre for Theoretical Physics, Trieste

8-11 December 1975

SUMMARY REPORT

Edited by

J.J. Schmidt

Nuclear Data Section
International Atomic Energy Agency
Vienna, Austria

March 1976

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Foreword

This meeting, recommended by the International Nuclear Data Committee (INDC) and convened by the IAEA Nuclear Data Section in cooperation with the International Centre for Theoretical Physics (ICTP) in Trieste, had the objectives to review the status and the use of nuclear theories, models and computer codes in the evaluation of neutron nuclear data needed for fission and fusion reactor design and other nuclear applications and to work out recommendations for future developments, with particular consideration of the requirements and possible cooperation of nuclear scientists from developing countries.

This report summarizes the major technical results and recommendations of the meeting. It consists of two major parts. The first part states the purpose of the meeting and the needs for improvement and contains also the general recommendations (chapters A, B and C), while the second part contains detailed technical reports and recommendations on each of the major topics dealt with at the meeting (chapter D). The report is followed by the list of working groups (Annex I), the list of review and contributed papers (Annex II), the meeting programme (Annex III) and the list of participants (Annex IV).

The meeting clearly demonstrated the importance of current research in basic nuclear theory for an improved understanding and determination of nuclear model parameters, a more adequate and detailed description of nuclear properties and reactions and thus for improvements in the prediction of neutron nuclear reaction data needed in nuclear energy applications. Eight review and twenty contributed papers presented in plenary followed by working group discussions formed the basis for a detailed review of the current and required developments in the following areas of nuclear theory:

- resonance and statistical theory;
- capture mechanism;
- nuclear level densities;
- optical model;
- pre-compound decay; and
- fission theory;

including a survey of available and required nuclear model computer codes. The meeting was thus in keeping with the traditional nuclear theory activities of the ICTP.

The most important result of the meeting is ~~therefore~~ the recommendation of an extended seminar of several weeks duration on nuclear theory and nuclear model computer codes for applications to be held in 19 7. As appropriate places the meeting suggested the ICTP in Trieste for the nuclear theory part, and the Centro di Calcolo of CNEN in Bologna or the NEA Computer Program Library at Ispra for the computer code part of the seminar.

The meeting was attended by 39 representatives from 16 countries and three international organizations. The excellent assistance by staff from the ICTP and the Institute of Theoretical Physics of the Trieste University contributed greatly to the success of the meeting and is most gratefully acknowledged.

The review and contributed papers written specifically for this meeting will be published separately as part of the IAEA-report series.

Summary report

A. INTRODUCTION

Following a recommendation by the International Nuclear Data Committee (INDC), the IAEA organised a Consultants Meeting at the International Centre for Theoretical Physics (ICTP) in Trieste from 8 to 12 December 1975 on the following subject:

"Use of Nuclear Theory for Neutron Nuclear Data Evaluation".

It is a well-known fact that neutron nuclear data are widely used for applications, the most important ones being at present related to nuclear energy. A world-wide network has been set up to gather the needs for such data which are compiled regularly in issues of WRENDA (World Request List for Nuclear Data). The needed data are obtained both from experiments and calculations based on nuclear theory and then transmitted to the users in the form of recommended or "evaluated" values in the appropriate format.

The purpose of the meeting was to examine one major aspect only of the whole chain of the production and use of nuclear data for applications, namely the contribution of the nuclear theory to the calculations of some of these data through the use of appropriate nuclear models and reaction mechanisms. In particular, the meeting did not cover other important aspects such as the assessment of the data needs or the evaluation of nuclear data directly from experimental results, because these topics were not relevant to the subject of the meeting. However, the participants took into account experimental results in addition to nuclear theory when it was necessary; for example to check the validity of the calculational method or to adjust the parameters of the theoretical models in cases where it is not possible to derive them from fundamental nuclear theory.

B. Need for Improvement

The meeting was organised in the form of a series of review papers and contributed papers, the presentation of which generated very useful discussions. These deliberations led to the definite conclusion that there are many areas in theoretical nuclear physics that should be expanded to meet the needs of the community of evaluators and users of nuclear data. The necessity of basic nuclear physics research was illustrated in numerous examples. Indeed the results of current fundamental research are being used to improve nuclear data evaluation. The physicists who are responsible for the recent development of nuclear models should be better informed by the evaluators of the usefulness and application of their work. In turn the evaluators are urged to express their needs in the field of nuclear theory as well as experimental nuclear physics.

While the area of expansion for a more thorough understanding of the fundamentals of nuclear structure and reactions is rather broad, some of the more important specific areas which would best benefit from developments in basic research should include:

(a) An improved microscopic interpretation of the optical model (e.g. parameter ambiguity, deformation effects, etc.);

(b) Various reaction mechanisms (e.g. (n, particle), and radiative capture reactions, pre-compound reactions, direct interactions, fission, etc.);

(c) Further development in the analysis of intermediate structure (e.g. doorway state concept; this is of special significance in the analysis of the neutron nuclear data of the important structure materials used in both fission and fusion reactors);

(d) Substantiation of parameterizations that are employed in many theoretical concepts, e.g. nuclear level densities, and a better fundamental understanding of the semi-empirical nature, approximations and the range of validity;

(e) Incorporation of nuclear structure concepts (e.g. shell model interpretation of level densities).

It was also recognized that investigations of nuclear reactions induced by particles other than neutrons (photons, charged particles, etc.) are also relevant to nuclear data applications to fission and fusion reactors.

It became clear during the discussions that the ideas and concepts of both basic and current physics should play a more active role in the interpretation of the fundamental data needs which can be brought about by establishing a closer communication between basic physicists and evaluators working in common areas.

Also, examination of the various calculational methods used to predict the cross sections has shown that the parameters used in the calculations cannot be derived from pure nuclear theory in its present stage but need to be adjusted to carefully selected experimental data. Therefore, in the foreseeable future, evaluation will still have to rely on good experimental results which, on the other hand, are the only way to obtain a large amount of the needed data with the required accuracy. Thus, it is clear that the developments in nuclear theory cannot replace the efforts made in experimental nuclear physics but rather supplement them.

C. General Recommendations

In the following the general recommendations following from this Consultants' Meeting are outlined. They are followed by detailed technical reports and specific recommendations which have been prepared by seven technical working groups during the meeting and approved by the plenary meeting. They cover the various technical aspects of nuclear theory and its applications in each of the fields mentioned under B. Details on the working groups are given in Annex I.

Having identified in section B the areas in which developments are required the meeting participants are of the opinion that, as a concrete first step towards initiating the required developments, an extended seminar of several weeks duration should be held at an appropriate future time (preferably in 1977) which will center on a few topics selected from the list given in section B, namely:

i) Nuclear level densities;

ii) Foundations and parameterization of the optical model;

iii) Pre-equilibrium mechanisms, including doorway state concepts;

iv) Fission theory; and

v) Intercomparison and development of relevant computer codes.

The consultants recommend to the IAEA to investigate the feasibility of holding such a seminar at a propre venue. From its tradition and experience of holding such extended seminars in nuclear theory at an international level and its particular ties with physicists in the developing countries, the ICTP in Trieste may be considered an appropriate location for the part of this seminar dealing with nuclear theory. For the second part dealing with computer codes the Centro di Calcolo of the Comitato Nazionale per l'Energia Nucleare in Bologna or the Computer Programme Library of the OECD Nuclear Energy Agency at Ispra would be appropriate places.

The primary purpose of this seminar would be to bring basic nuclear theorists and nuclear data evaluators together to discuss the state of the art in each field and to point out the needed developments. It was realized from the discussions of the consultants meeting that the need for interaction between basic theorists, data evaluators and users is greater for developing countries. By ensuring an appropriate participation from the developing countries both at the lecturers and participants level, the seminar would also partially fulfil this need. It is understood that a possible outcome of the seminar, apart from initiating the required research programmes in nuclear theory, would be recommendations as to further actions necessary to continue the manpower training aspects relevant to developing countries.

If the recommendation to hold this seminar is accepted an organizing committee should be nominated by the IAEA as soon as possible so that the framework and the detailed structure and programme of the seminar can be worked out during 1976.

D. Technical reports and recommendations

Authors, titles and numbers of review papers (RP) and contributed papers (CP) referenced in this chapter are contained in Annex II.

D.1. Resonance and statistical theory

1. General

The resonance and statistical theories of neutron cross sections are formalisms that permit one to connect the values of parameters of certain physical models with properties of neutron cross sections. As such they are important means for the interpolation and extrapolation of measured cross sections and the estimation of unmeasured ones [RP 1a, RP 2]. Their most important applications pertain to the areas of design and operation of fast fission breeder reactors and, to an increasing measure, fusion reactor research and design.

2. Resonance theories

At low neutron energies and in very light nuclei the neutron cross section behaviour can be expressed in terms of Breit-Wigner resonances and the parameters of resonance energies, resonance total and partial widths. Statistical theories of the distributions and correlations of these quantities are well established. Their specific values must in general be determined by the fitting of cross section data. Efforts to determine these properties from nuclear structure calculations using the continuum shell model theory were reported in paper CP 3.

At slightly higher neutron energies the resonances begin to overlap and often more than one competing channel is open. In that case the most appropriate method for parameterizing the detailed energy dependence of the neutron cross sections is the multilevel multichannel R-matrix method. This method can be used with few approximations to give a rather complete and detailed description of nuclear data from reactions in light systems where the number of channels and levels is manageable [CP 1]. Approximations, such as those given by Reich and Moore and by Adler and Adler, can be used to treat large numbers of channels and levels without introducing significantly more parameters. Numbers of required parameters quickly increase to unmanageable proportions as the neutron energy increases and as a detailed description becomes less important in applications.

3. Statistical theory of average neutron cross sections

At higher energies, applications in general require mostly energy averaged cross sections [RP 2]. These are quite generally represented by the Hauser-Feshbach formula with a fluctuation correction factor. The parameters required are channel transmission coefficients obtained from the optical model and channel fluctuation indices (chi-squared degrees of freedom) that enter into the fluctuation correction. Empirical formulas connecting these fluctuation indices with transmission coefficients are generally successful, but further theoretical and empirical work for their determination is required. An approximation to the fluctuation correction that does not require the evaluation of an integral is satisfactory over a wide range of parameters but fails sometimes for reactions between weakly absorbed channels. Alternate approaches to the average cross section theory that have recently been proposed merit further study and evaluation.

In the presence of competing direct reactions the average cross sections can be computed from the reaction amplitudes [RP 5] of coupled channel models and the fluctuation indices by means of the Engelbrecht-Weidenmueller transformation. Though this effect of competing direct reactions in enhancing the average value of the fluctuating cross section can be pronounced it is expected to occur only in rather limited circumstances. More widely applicable effects occur in polarization phenomena and in fluctuation phenomena.

4. Averaging intervals and doorway states

In statistical theory one presupposes the choice of an energy interval. These averaging intervals are determined either by the experimental resolution or by the energy group structure used in applications.

The relationships between statistical assumptions and sizes of averaging intervals require further study and elaboration. This is particularly important to the problem of assigning reliability to computed group cross sections. In this connection the relationship between statistical theories and doorway state phenomena such as pre-equilibrium processes [RP 6] require further study.

5. Statistics of cross section fluctuations

For some applications a statistical description of the fluctuations (such as Ericson fluctuations) of scattering cross sections about their averages is important. This applies particularly to the estimation of the probability of the occurrence of flux "windows" due to very deep minima of the scattering cross sections. Old existing theories of cross section fluctuations need to be reexamined in the light of recent developments in the statistical theory of average cross sections.

6. Particle emission spectra and tertiary reactions

6.1. Particle emission spectra

Particle emission spectra are calculated with compound theories, supplemented with pre-equilibrium and/or direct reaction models. Since a number of papers presented at this meeting deal with pre-equilibrium models we refer to the conclusions presented in chapter D.5.

6.2. Tertiary reactions

In view of the growing interest in fast neutron dosimetry and CTR applications tertiary reactions are becoming more important. Several papers deal with these reactions [RP 1a, RP 6, CP 12, 13, 17 and 18]. The treatment of these types of reactions is straightforward when only Hauser-Feshbach theory is used. However, in many cases pre-compound processes and direct reaction models have to be taken into consideration [RP 6, CP 12 and 13, and chapter D.5.].

The paper of Uhl [CP 17] describes a code which can handle a large variety of tertiary reactions including γ-ray cascade emission. Some unusual features of this code are: the use of "discrete" level schemes as far as possible at all stages of the decay, the use of E1, M1 and higher multipole radiation strength functions (Brink-Axel and/or Weisskopf estimates) and the inclusion of pre-equilibrium processes.

Matthes' paper [CP 18] describes a code in which all tertiary reactions (i.e. the complete nuclear decay cascade) are treated in one computer run.

7. Parameter sensitivity and cross section uncertainty

7.1. Uncertainties in model parameters often are the most important sources of errors in the cross sections as calculated with the statistical model. One important reason for these uncertainties is that all the parameters of statistical theories are ultimately derived from experimental data representing finite samples. Very often these samples are very small. The status of the knowledge of these parameters might be summarized as follows:

7.1.1. Neutron transmission coefficients and strength functions

The present global optical model parameter sets [RP 5] do not adequately describe many types of cross sections important for applications. A more thorough optical model analysis of all available experimental data for each nuclide is required in order to be a reliable statistical description of all relevant cross sections of that nuclide.

Thus one might hope to be able to describe all cross section types for one nuclide in a satisfactory way. One useful approach is the so-called SPRT-method [RP 5] which has the advantage that the s- and p-wave strength functions, the potential scattering radius and the total cross section are constrained to the experimental values in the fitting procedure. This would indeed be very valuable for evaluation purposes as one could avoid the use of two different models (i.e. strength function model and optical model).

7.1.2. Nuclear level density parameters

The nuclear level density is a very important quantity in the statistical theory as it affects the γ-ray strength, the fission strength and inelastic scattering in the continuum. The uncertainty in the nuclear level density is a basic limitation of the application of statistical theory. A new semi-empirical formula has been suggested by Ramamurthy et al. [CP 6]. Jensen [CP 5] uses a more basic approach, but still the results are not sufficiently precise for cross section predictions (see further conclusions presented in chapter D.3.).

Other uncertainties in the cross section arise from uncertainties in the spin and parity distribution of bound and unbound states [CP 4].

7.1.3. "Gamma parameters"

In nearly all cross section calculations the Brink-Axel estimate is used for the calculation of the E1-radiation strength function. For deformed nuclei two Lorentz curves are required in general [CP 2]. When giant resonance parameters are extracted from photon absorption cross sections one only has to take into account the $T_<$ (isospin) component, since the $T_>$ component is not excited in neutron reactions [CP 2]. For M1-radiation Uhl [CP 17] uses the Weisskopf estimate.

In many cases the γ-ray strength function is normalized to the experimental value at the neutron binding energy. Therefore, the parameters $\Gamma_\gamma^{\ell=\mathrm{even}}$ and $\Gamma_\gamma^{\ell=\mathrm{odd}}$ are important quantities in the calculation of the capture cross section. Difficulties in the experimental determination of these parameters might arise from unknown parities of unresolved resonances or from non-statistical effects (e.g. valence capture) [CP 4]. The theoretical calculation of Γ_γ is difficult mainly due to uncertainties in the density, spin and parity distribution of levels.

7.1.4. Fission parameters

See chapter D.6. and RP 1a, RP 7, CP 19 and CP 20.

7.2. Uncertainty calculations

Uncertainty calculations (including the calculation of covariances) have been performed for the capture cross sections of a number of fission-product nuclides [CP 4]. Some conclusions are:

(i) parameter uncertainties are generally the most important source of uncertainties,

(ii) uncertainties arising from the statistical nature of the model are important when the model is applied at very low energies or when very little is known about the bound target nucleus levels.

8. Applications

The statistical model is one of the most powerful tools in cross section evaluation and prediction. It is used in almost any cross section evaluation. The model is in particular useful to predict data in mass ranges where not much data are known from experiments, such as in the fission product mass range [CP 4], the actinide mass range [CP 8] or data for fusion applications [CP 12, 13 and 14].

9. Recommendations

The meeting participants recommend work and further international discussion on the following topics:

9.1. Evaluation and generalization of new approaches to the theory of average cross section and fluctuations;

9.2. The relationships between various reaction mechanisms (direct, compound, pre-compound and doorway states) and the statistical theory of nuclear reactions.

9.3. Nuclear level density including spin and parity distributions;

9.4. Derivation of optical model parameters from all available experimental data with emphasis on low-energy neutron data;

9.5. Calculation of γ-ray widths including direct effects;

9.6. Application of fission theories (see chapter D.7.); and

9.7. Sensitivity and uncertainties of group cross sections.

The meeting participants recommend the development of computer codes for the following subjects:

9.8. Hauser-Feshbach theory including generalized width fluctuation factors and γ-ray and fission channels and charged-particle emission. Provisions should be made for the inclusion of direct and pre-compound effects and the Satchler penetration matrix should be calculated by coupled channel and other direct reaction programmes.

D.2. Capture mechanism

The capture cross sections and γ-ray spectra from capture reactions of low-energy neutrons are of importance in fission reactor design. For fusion reactors the neutron energy range of interest extends to about 20 MeV.

At low neutron energies the compound-nucleus theory is generally applicable and the concept of γ-ray strength function is introduced. A simple description of the γ-ray strength function is obtained by extrapolating the giant-dipole resonance strength to lower γ-ray energies (Brink-Axel approach). This method is discussed in paper CP 2. This approach has been tested experimentally for some nuclei with mass number $A \geqslant 90$. It has been observed that the model provides a good description of the γ-ray strength in a number of cases, but serious discrepancies occur for several nuclei. More experimental work is needed to better establish the systematics of the γ-ray strength for heavy nuclei as well as for nuclei with $A < 90$. More theoretical work is necessary to understand present discrepancies between theory and experiment.

At high neutron energies (5-20 MeV) the direct-semidirect model has given a generally satisfactory explanation of experimental data. However, the best form of the particle-vibration coupling interaction which should be used is still an open question [RP 3]. A possible contribution to the (n, γ) cross section by the compound nucleus mechanism seems the best way for removing some of the remaining discrepancies. It should be underlined that the results of direct-semidirect model calculations are highly dependent on the values of the bound, optical and giant-dipole state parameters used. This specially refers to the crucial parameters such as the strengths of the isospin part of the optical potential. Knowledge of the spectroscopic factors and level schemes for the nuclei considered is also important in obtaining accurate results. Therefore, it seems that the determination of reliable parameter sets obtained on the basis of systematic analyses of large amounts of data remains the main direction towards which the efforts of evaluators should be directed.

D.3. Nuclear level densities

In all calculations of neutron cross sections for applied purposes the nuclear level density is one of the most important parameters.

The intrinsic nuclear level density, i.e. the level density arising from excitations of the intrinsic degrees of freedom, is well defined in terms of the single particle energies E_i. However, the E_i to be used for the particular case considered cannot be specified uniquely. Different average potentials may be used for the E_i-calculations, i.e. Nilsson-type potentials, Woods-Saxon potentials, etc.

From the intrinsic level density the total level density should be derived. This has been done traditionally without considering contributions from collective states, but has proved inadequate.

Rotations should be included for deformed nucei at low excitation energies. Comparison of observed level densities at the neutron separation energy with calculations from different single particle spectra indicate an uncertainty of around a factor of 5 in the estimates. This uncertainty assumes that all contributing degrees of freedom are included.

A number of theoretical difficulties still remain, e.g. how to treat

1) the transition region between spherical nuclei, where rotations do not contribute, and deformed nuclei, where rotations should be included for low excitation energies;

2) the transition for deformed nuclei between low excitation energies, where rotations should be included, and higher excitation energies, around 50 MeV where the rotational contribution is already included in the intrinsic level density; and

3) other collective states, e.g. vibrations, and their contributions as a function of energy.

For application purposes the uncertainty given above is completely unacceptable. Instead of using absolute calculations the level density has consequently been parameterized by simple expressions. The parameters are taken from systematics of observations or adjusted to the particular situation considered. Extrapolations are then obviously very dangerous because the form of the expression may not be generally valid.

To obtain better level density expressions the theory should be used to give the functional dependence in an analytical form. Then the parameters entering should be adjusted to the energy region and the nuclei under consideration. Examples of this procedure are outlined in papers CP 5 and CP 6.

Summarizing it is very essential to have the guidance from theory. One should therefore investigate theoretically the level density problem. This leads presumably first to more uncertain estimates but we obtain knowledge about the essential effects and the regions where they are important. From this one may proceed empirically or phenomenologically with adjustable parameters in the theoretical expressions.

D.4. Optical model

Together with resonance, statistical, pre-equilibrium and direct nuclear reaction theories, the optical model belongs to the most important tools of nuclear theory for the interpretation and prediction of neutron cross sections for applied purposes.

The optical model is often the basis of other theories, and a knowledge of the optical potential is needed for their discussion. In general good methods have been developed to deal with the parameters in the optical potential and the user may choose between the use of global optical potentials which have been developed to give overall descriptions of nuclear scattering problems, and more detailed potentials which apply only over a small range of nuclear mass and energy. Thus, if a rough estimate of cross sections is sufficient, then global potentials may be used, but for more accurate results it is necessary to use potentials fitted to carefully selected experimental data.

In order to predict a coherent set of cross section data with enough accuracy over a wide range of energy for a given nucleus (or a family of neighbouring nuclei), it is recommended that a set of optical potential parameters is determined for each individual nuclide. The recommended basic physical criteria for such determinations are the strength functions, the scattering radius at neutron binding energy and the total cross-sections over the full energy range.

A great amount of work has aimed at obtaining a good understanding of the optical potential, and the present description is on the whole satisfactory, but there are several gaps in our understanding. One is the role of the isospin potential. Here, experiments using the scattering of protons can give information leading to an improved isospin term for the optical potential. This is needed for regions such as those far from the nuclear stability line (e.g. fission products and actinides) and which cannot be reached by experimental techniques. It is thought that unlike the spherical optical potential, the deformed nuclear model still has some areas where development is necessary. More accurately known deformation parameters are needed. These should not be derived from the scattering theory itself, but should be obtained from other sources. Thus the Nilsson model or the Hartree-Fock method could be used and the results of experimental investigations of phenomena such as Coulomb scattering can also be taken into account. Another deficiency of the present theory is the usual neglect of more complex collective states than purely vibrational or purely rotational levels. Future work is needed to obtain a better understanding of the nuclear structure of low-lying states so that nuclei such as the transitional elements can be well described. Another future development can be envisaged to be the use of microscopic models to give direct derivations of the optical potential for each nucleus. In this field particularly, recent methods of parameterizing the optical model in a matrix form should prove useful.

The present needs for optical model calculations for nuclear data evaluation purposes are not always well met by the available computer codes. In particular more flexibility in the use of input and output data would be very useful. Also, developing countries often have limited computing facilities, and perhaps more suitable codes could be developed to meet their needs. To this end, tables of commonly used functions and parameters such as the transmission coefficients from a standard set of global optical potentials should be prepared. These could be used directly in the calculations of other quantities, such as the compound inelastic scattering cross sections, in establishments with limited computing facilities. In cases where such a set of tables would be insufficiently accurate, sets of optical potentials for specific nuclei could be used. To facilitate such a use it is recommended that a compilation should be made of proposed optical potential parameters as a function of mass number.

It is recommended that a seminar on the optical model should treat the following topics:

1. Foundation and theory of the optical model;

2. Conventional and new methods for the solution of the equations for spherical and deformed optical potentials in different representations;

3. Optical potentials, their phenomenological and fundamental basis including non-local effects, folding potential, and parameterization procedures;

4. Applicability of the model, its range of validity and use in evaluation.

The major emphasis should be on the numerical aspects, the application of the model and its range of validity. The other topics should be included only in such detail as to enable a sufficient understanding to be developed.

D.5. Pre-compound decay

The concept of the pre-compound decay mechanism turned out to be necessary for the description of neutron and charged particle induced nuclear reactions for incident particle energies above 5 MeV. In particular it was shown [RP 6, CP 12, 13, 14, 15 and 17] that existing modifications of the exciton model are able and necessary to describe in an absolute manner the following experimental observations:

- the high energy part of neutron emission spectra;
- the excitation functions of all kinds of neutron-induced reactions; especially pre-equilibrium emission turns out to be a dominating process for charged particle emission (reactions (n,α), (n,p) from heavy nuclei; and
- the cross section values and particle spectra of tertiary reactions such as (n,2n) and (n,pn) reactions.

The progress achieved in the development of exciton models recommends their application to neutron data as it was shown for the case of ^{93}Nb [CP 14]. A proper description of the γ-decay within this model and its influence on the fission mechanism is not as well developed.

A complete justification of the pre-compound model from basic nuclear theory has not yet been obtained. The model, however, is so simple and successful that a further elaboration is highly desirable as it allows predictions and calculations of reaction cross-sections and particle spectra for important practical applications (e.g. activation cross sections for threshold reactions as needed for reactor neutron dosimetry, the prediction of radioactive contamination of reactor structure materials and for radioisotope production; a knowledge of the pre-compound component of secondary neutron spectra is required for a more accurate treatment of

a) Breeding problems in fusion reactors,

b) Shielding in fusion and fast fission reactors, and

c) Inner wall problems in fusion reactors).

The problem to give the model a sound theoretical foundation is just as important as it

a) will help to clarify the distinction between direct and pre-compound nuclear reactions;

b) improve the understanding of the effects of nuclear structure on the pre-compound decay and the process of energy dissipation in a complex system such as a nucleus; and

c) provide the possibility for a correct treatment of angular momentum in the pre-compound phase in nuclear model codes.

In spite of the simplicity and the success of this model many important questions for a deeper understanding of the pre-compound mechanism are still open. To fill this gap well defined experiments such as

a) investigations of charged particle and neutron reactions (e.g. (p,n), (p,p'), (n,p), (n,pn)) with a better energy resolution to enable a clear separation of the pre-compound component from the observed particle spectrum; and

b) Pion capture experiments (as these experiments establish a well defined initial condition for a nucleus decaying into the pre-compound mode)

will help to resolve the open problems.

To stimulate further research in this field expert lectures on this topic are recommended for the nuclear theory seminar proposed for 1977 (see chapter C).

D.6. Fission theory

1. Importance and applications of fission theory

Measurement of nuclear data to the accuracy required for many technological purposes is notoriously difficult, particularly for neutrons and gamma rays, both these quanta being detectable not directly, but only through secondary charged particle production in the detector medium. As examples of the scale of the difficulties, decades of work have resulted in the cross-sections of the three commonest fissile nuclides being known to better than 1% only for neutrons of velocity 2200 ms^{-1}, while the energy-dependent fission cross sections of fast neutrons of ^{235}U, ^{239}Pu and ^{238}U are now known to between 3 and 5%, whereas for reactor physics purposes an accuracy of better than 1% is desirable; and these are nuclides for which high quality samples are readily available for experimental measurement. In all countries there are now severe economic constraints on the amount of effort that can be put into nuclear data measurements, while at the same time the range of nuclei for which sophisticated data are required is increasing rapidly.

Apart from the few actinide nuclei which have already been measured to a considerable degree of accuracy (^{235}U, ^{238}U, ^{239}Pu, possibly ^{233}U and ^{232}Th) data on many higher trans-plutonium, trans-uranium and trans-actinium nuclei are required for such purposes as:

a) Build-up of such nuclei and change of reactor physics characteristics in the course of long reactor operation;

b) Operations (such as transport) and processing plant design for spent fuel;

c) Considerations on the viability of long-term future schemes for the nuclear incineration of the higher actinides produced as "waste" from large scale nuclear power programmes.

For all these aspects not only cross section data but fission product yield data are vitally important. The details of the requirements need not be stated in detail here, for they have been discussed, and summaries of conclusions and recommendations have been produced at the recent IAEA Advisory Group Meeting on Transactinium Isotope Nuclear Data held at Karlsruhe in November 1975. (Proceedings to be published).

Clearly it is not going to be possible to provide the bulk of such data from experiment in the readily foreseeable future, especially as many of the nuclides for which data are required are either very difficult to obtain in suitable form or are so radioactive that the desired measurement cannot readily be carried out; the transactinium nuclei and the fission products are outstanding examples of this.

2. Status of fission theory

There has been a tremendous surge of activity in the field of fission theory since the work of Strutinsky and the discovery of the double-humped fission barrier in 1967. Yet, in spite of all this work and advance, fission theory as such has not yet achieved the state of quantitative accuracy in which it can be used, starting entirely from basic principles, to provide useful data for the compilations needed for technology.

The main role of fission theory in nuclear data evaluation at present is to connect and systematize a variety of experimental data, including non-neutron nuclear reaction data and nuclear structure data. (For instance, it is possible that experimental work in such apparently exotic matters as muon- and meson-induced fission could be relevant). It can thus reveal parameterizations which can be used with reasonable confidence in quantitative calculations.

Fission theory work at present is following three main tracks:

a) mapping-out of potential energy surfaces in deformation space;

b) dynamic considerations including inertial parameters; and

c) study of the role of viscosity and related statistical models.

The general status of each of these is as follows:

2.1. Potential energy surfaces

We remark first that different theoretical schools each tend to employ their own parameterization of deformation space. Thus intercomparison of results is difficult, and the work so far done is not guaranteed to be physically complete, because the deformation space explored is limited and to some extent distorted by the parameter choice, which is itself limited for practical computational reasons.

From the calculations available up to now on the fission barrier region, uncertainties of the order of 1/2 to 1 MeV in the estimation of barrier heights seem to be inherent at the present stage of theory. These correspond to uncertainties of the order of factors of 3 to 10 in the calculation of fission cross sections.

For mass yield determination the potential energy surface between the barrier and the scission point is important. The remarks made above on the barrier region are emphasized here *a fortiori*, since this region of deformation space is much more complicated and has been much less thoroughly explored.

2.2. Dynamical considerations such as inertial parameters

All investigations so far have employed the cranking formalism; the basis of the cranking formula and its sufficiency need to be further explored. Most work has been devoted to ground states, rather than to excited states. The conclusion is that this work is still in an early phase and cannot be used effectively for predicting data.

2.3. Viscosity etc.

This is an even more preliminary phase (as far as basic work starting from microscopic theory is concerned). Here it is necessary to connect with theories being studied in heavy-ion reactions. More immediately, it seems most profitable to obtain information on nuclear viscosity (and on special aspects of it such as superfluid flow in very low energy fission) from a study and analysis of fission product mass, charge and excitation energy yield data, using statistical models for the later stages of the fission process.

Thus, theoretical considerations starting from basic principles are unable to produce data of the kind of accuracy required in applications, but show promise of eventually being able to do so. However, applications of the present theoretical understanding of the fission process to the analysis of experimental data allows parameterizations and calculational schemes to be developed which will allow the prediction of many cross sections, for example, to an accuracy probably of the order of 30%. Such studies also have relevance to the energy dependence of $\overline{v}$. In evaluations it is co[illegible] to extrapolate this quantity in a linear manner from the values for thermal neutron-induced fission and spontaneous fission, but the increasing recognition of the influence of superfluid flow in fission at low excitation energies makes this an unsafe procedure.

3. Some recommendations for specific future work

The foundations of models for calculating many cross sections related to fission have already been laid. These now require extension and consolidation. In particular the present schemes are weakest for the low-charge (thorium region) nuclei in the actinide set. The cross sections of such nuclei are characterised by strong vibrational resonances, implying that the inner and outer barriers are rather close in magnitude and that the secondary well between them is shallow. The main body of theory on potential energy surfaces does not reproduce this feature, so at present the parameterization of the fission barriers of the low charge nuclei is not solidly backed by fundamental theory. Two hopes for improvement come from the work of Nix and Moeller on the one hand, suggesting that the outer barrier is itself split giving a shallow third minimum, and of Larsson et al on the other, implying that the quadrupole pairing force will appreciably raise the inner barrier for the lighter nuclei. Further very careful exploration of the potential energy surfaces of these nuclei is required, and the associated fission reaction theory arising from new phenomena like a third minimum in the barrier needs to be developed. In this connection the shape symmetry needs careful attention so that the correct level density formulae and low-lying channel structures for the calculation of barrrier transmission coefficients are used. Such barrier level density calculations, and the associated statistical questions of coupling the barriers in the high temperature limit (thermodynamic models suggest the reversion of the barrier to a single hump at high temperatures), need to be extended to high excitation energies so that (n,Xn) and (n,XnF) cross sections can be treated with confidence. Barrier penetrability formulae need further consideration; the Hill-Wheeler formula is almost certainly too simple, and further work along the lines of the two-dimensional fission barrier models of Hofmann and Massmann et al may well be valuable. At the same time important developments are required in aspects of reaction theory apart from fission. These concern radiative de-excitation mechanisms, compound nucleus formation cross sections, and coupled-channel aspects of inelastic scattering; the present status of these matters is summarized in papers of the Karlsruhe Transactinium Isotope Nuclear Data Meeting and also of this meeting.

Although a fully developed basic theory of fission product yields is not likely to appear for some years, it would seem both necessary and possible for theoretical development (both from potential energy calculations and statistical models) to be made to support some of the semi-empirical work on yields that is now being used in the data application field.

Apart from the matter of cross sections, the most likely area where fission theory may throw new light concerns the fission neutron spectrum. Data are either lacking or poor for fission neutron energies below 100 or 200 keV, these data are important for an understanding of fast reactor physics relating to such matters as breeding ratios and Doppler temperature coefficient of reactivity. The mathematical forms adopted for describing fission neutron spectra are only suggested by nuclear theoretical ideas, rather than being rigorously based on them, and hence are suspect for the purposes of extrapolating the spectra down to very low energies. A proper theoretical treatment of this problem would have to await a full theory of mass and energy distributions, which is likely to be some time distant. Yet there are still useful contributions that fission theory can make on a shorter time-scale. One is a firmer appreciation of the role of neutrons emitted at or near the scission point. No serious theoretical work on the likely fraction or energy distribution of scission neutrons seems to have been attempted. A possible start in this direction could be based on the potential energy surfaces at extreme deformation now being developed using the Strutinsky method; with allowance for a phenomenological temperature for intrinsic excitation the population of unbound neutron levels and their emission probability might be estimated. There is certainly a great deal of scope for much more sophisticated phenomenological analysis of the great body of experimental data on neutron and gamma-ray emission in the fission process.

4. Status and requirements for computer codes

4.1. Strutinsky method

From the literature it is known that many codes based on the Strutinsky method of calculating potential energy surfaces are in existence. These employ a variety of different nuclear shell models and shape parameterizations. However, they do not seem to be generally available. Efforts should be made to encourage the authors of these codes to make their work freely available, but at the same time it would be advisable that some effort is made on duplicating or cross checking some of these programmes. There are also related computer codes available for calculation of inertial parameters.

4.2. Codes for fission cross section calculations

A few codes are known to exist (e.g. at Harwell and Los Alamos) for treatment of fission widths, fission transmission coefficients etc. within the framework of the double-humped barrier. These employ either empirical or calculated level density formulae. Such formulations, particularly for barrier level densities, are still in course of fairly rapid development, so because of this it will likely take quite some time before the codes become freely available. Related codes that will be of value in this field are level density codes, known to exist at many laboratories. New developments in those that are desirable and should eventually be included are the incorporation of rotational and other collective enhancement factors due to asymmetry of nuclear shapes.

4.3. Codes for nuclear fission theory

In general, there seems to be no general collection of knowledge about the existence of computer codes specific to nuclear fission theory. This contrasts with the situation in other fields of nuclear reaction theory relevant to nuclear data evaluation, for which quite extensive lists and information, and even complete codes, have been collected, for example at Ispra and Bologna. We recommend, therefore, that a specific organization represented at this Consultants' Meeting be appointed to make a systematic search for such information.

5. Recommendations for further procedure

At present there is still such a momentum in fission theory, following the Strutinsky "revolution", that it can be safely expected that a number of further developments will take place in the immediate future. In addition, however, a focusing of the work in fission theory onto its applications for nuclear data evaluation is now required. This we feel can best be achieved at the extended seminar recommended to be held at the ICTP in Trieste in 1977. In this connection we note that the next International Symposium on "Physics and Chemistry of Fission" organized by the IAEA is also planned to be held in 1977. Since many of the world's leading experts in fission theory are bound to be present at this Symposium, we recommend that the Seminar be held immediately following the Symposium, so that many of the experts can take part in the Seminar, and the new ideas and results from the Symposium can be exploited by the Seminar.

D.7. Nuclear model computer codes

1. Status, testing and documentation of computer codes

Since the 1971 IAEA Panel on Neutron Nuclear Data Evaluation, when a volunteer effort on a world-wide basis was suggested for comparing results obtained from different codes treating the same physical problem, a number of such comparisons were carried out [RP 1a].

The meeting participants recommend that these inter-comparisons be continued on a volunteer basis (for example in the fields of coupled channel models with particular attention to penetration matrices, precompound model calculations and codes for the calculation of non-neutron nuclear data for energy applications).

Such actions should possibly be encouraged by the IAEA by informing the institutions concerned in the various countries - through the liaison officer circuit - of the efforts underway so that contributions are received from different countries and maximum efficiency can be achieved through the exchange of information and experience.

2. Availability and dissemination of computer codes

Since the recommendations made at the above mentioned IAEA Panel in 1971, lists of existing and available codes were published and distributed by the OECD Nuclear Energy Agency (NEANDC-97/U). The meeting recommends that appropriate actions be undertaken in the various organizations concerned (i.e. national nuclear data committees) so that the quality of this list is improved in the following points:

- whether the code is still used and gives acceptable results;
- whether the code is obsolete and by which code it is superseded;
- which additional codes should be included in the NEA Computer Program Library collection; and
- by adding names of additional codes which are considered to be of interest to the user community.

The meeting participants feel that the publication of a bulletin containing information on developments and adaptations to different computers of codes in the field of nuclear model calculations would greatly improve the exchange and dissemination of the codes. This would be especially beneficial to those research centres, which have access to only small and medium size computers. The meeting recommends that the necessary steps to create such a bulletin be taken up by the IAEA (in collaboration with the Computer Program Library, the United States Code Center and the Belfast Computer Physics Communication Program Library). From the practical point of view the working group suggests that a questionnaire on nuclear model codes, like the one proposed in the previously mentioned IAEA Panel (IAEA Technical Report Series No.146, p. 110) be circulated by the liaison officers of INDC and CPL.

3. Computer codes situation of developing countries

It became apparent that during the last years the needs and efforts in developing and adapting computer codes which can be used for nuclear data evaluation are increasing in those countries which have no access to large computers.

In order to minimize duplication of effort it is suggested that when developing new codes for big computers, programming techniques be used which facilitate the adaptation of these codes with minor modifications to smaller computers.

4. Seminar at the NEA Computer Program Library

The meeting feels that a short seminar on nuclear model computer codes would be useful for the preparation of the extended seminar on nuclear model computer codes recommended for 1977 (chapter C). An appropriate place for this preparatory seminar would be the NEA Computer Program Library. A proper time would be towards the end of 1976. Its purpose would be to review the status, availability and applicability of all those codes to be intercompared at the extended seminar in 1977.

List of working groups

Title	Chapter	Chairman	Secretary	Members
General recommendations	A, B and C	M.K. Mehta	A. Prince	I. Brandus C. Ertek A. Michaudon A. Rimini G. Ripka J.J. Schmidt
Resonance and statistical theory	D 1	P.A. Moldauer	H. Gruppelaar	G.M. Hale E. Menapace G. Reffo T. Weber
Capture mechanism	D 2	G. Longo	I. Bergqvist	I. Rotter
Nuclear level densities	D 3	A.S. Jensen		–
Optical model	D 4	J. Salvy	D. Wilmore	S. Igarasi Ch. Lagrange T. Wiedling
Pre-compound decay	D 5	D. Seeliger	W. Matthes	H. Jahn M. Uhl
Fission theory	D 6	J.E. Lynn	U. Facchini	E. Fort J. Hadermann N. Janeva A. Ventura
Nuclear model computer codes	D 7	V. Benzi	E. Sartori	F. Fabbri S. Igarasi A. Prince M. Visinescu

Annex II

List of review and contributed papers

A. Review papers (RP)

RP 1a A. Prince

The role and use of nuclear theories and models in practical evaluation of neutron nuclear data needed for fission and fusion reactor design and other nuclear applications.

RP 1b M.K. Mehta

The role and importance of the use and development of applied nuclear theory and computer codes for neutron nuclear data evaluation in developing countries.

RP 2 P.A. Moldauer

Statistical theory of neutron nuclear reactions.

RP 3 G. Longo and F. Saporetti

Radiative capture of 5-20 MeV neutrons.

RP 4 A.V. Ignatyuk

Statistical characteristics of excited nuclei.

RP 5 J.P. Delaroche, Ch. Lagrange and J. Salvy

The cptical model with particular consideration of the coupled-channel optical model.

RP 6 D. Seeliger

Pre-equilibrium emission in neutron induced reactions.

RP 7 J.E. Lynn

Fission theory and its application to the compilation of nuclear data.

B. Contributed papers (CP)

CP 1 G.M. Hale

R-matrix methods for light systems.

CP 2 I. Bergqvist

Photon strength functions.

CP 3 I. Rotter, H.W. Barz and J. Hoehn

On threshold effects in the statistical distribution of neutron capture widths.

CP 4 H. Gruppelaar

Uncertainty estimates of statistical theory calculations of neutron capture cross sections of fission products.

CP 5 A.S. Jensen

Uncertainties and applications of the nuclear level density with inclusion of collective rotations.

CP 6 V.S. Ramamurthy, S.K. Kataria, S.S. Kapoor

On a new semi-empirical nuclear level density formula with shell effects.

CP 7 D. Wilmore and P.E. Hodgson

Neutron optical potentials.

CP 8 S. Igarasi

Application of the statistical theory to the prediction and evaluation of neutron cross sections for reactors - evaluation of ^{241}Am cross sections.

CP 9 T. Wiedling, E. Ramstroem and B. Holmqvist

Systematic optical and Hauser-Feshbach model interpretation of measured elastic and inelastic neutron scattering data.

CP 10 T. Schweitzer, D. Seeliger, K. Seidel and S. Unholzer

Analysis of differential elastic and inelastic scattering cross sections by the Hauser-Feshbach theory.

CP 11 E. Sartori

Nuclear model codes available at the Nuclear Energy Agency Computer Program Library (NEA-CPL).

CP 12 D. Hermsdorf, A. Meister, S. Sassonov, D. Seeliger and K. Seidel

Neutron emission spectra analysis with pre-equilibrium and equilibrium statistical theory.

CP 13 K. Seidel, D. Seeliger, A. Meister

Calculation of pre-equilibrium processes in (n,2n), (n,np) and (n,pn) reactions.

CP 14 D. Hermsdorf, G. Kiessig and D. Seeliger

The use of the pre-equilibrium model in the evaluation of ^{93}Nb + n cross sections.

CP 15 H. Jahn

Absolute values, geometry dependent effects and the direct component in the pre-equilibrium analysis of inelastically scattered neutrons.

CP 16 E. Arndt and R. Reif

Direct inelastic nucleon scattering to higher excited states.

CP 17 M. Uhl

Computer calculations of neutron cross sections and γ-cascades with the statistical model with consideration of angular momentum and parity conservation.

CP 18 W. Matthes

The MODESTY-PL/1 programme for the calculation of nuclear reaction cross sections.

CP 19 U. Facchini and G. Sassi

A statistical approach to the scission mechanism.

CP 20 V. Benzi

Note on the neutron-fission competition in heavy nuclei.

Annex III

Meeting programme

Monday - Wednesday, 8-10 December

Presentation and discussion of review and contributed papers

Session 1 Introductory (Chairman: J.J. Schmidt)

Openings and announcements

Discussion of meeting programme

Election of working groups, chairmen, secretaries and participants

RP 1a Prince

RP 1b Mehta

plus discussion periods

Session 2 Resonance and statistical theory (including capture mechanism and nuclear level densities) (Chairmen:
first half: L. Fonda
second half: P.A. Moldauer)

CP 1 Hale

RP 2 Moldauer

RP 3 Longo/Saporetti

CP 2 Bergqvist

CP 3 Rotter et al.

CP 4 Gruppelaar

CP 5 Jensen

CP 6 Ramamurthy et al.

plus discussion periods

Session 3 Optical model (Chairman: V. Benzi)

RP 5 Salvy et al.

CP 7 Wilmore/Hodgson

CP 8 Igarasi

CP 9 Wiedling et al.

CP 10 Schweitzer et al.

CP 11 Sartori

plus discussion periods

Session 4 Pre-compound decay (Chairman: D. Seeliger)

RP 6 Seeliger

CP 12 Hermsdorf et al.

CP 13 Seidel et al.

CP 14 Hermsdorf et al.

CP 16 Arndt/Reif

CP 15 Jahn

CP 17 Uhl

CP 18 Matthes

plus discussion periods

Session 5 Fission theory (Chairman: A. Michaudon)

RP 7 Lynn

CP 19 Facchini/Sassi

CP 20 Benzi

plus discussion periods

Thursday, 11 December, day-time

Session 6	Working groups (WG)	
	WG 1	General recommendations
	WG 2	Resonance and statistical theory
	WG 3	Capture mechanism
	WG 4	Nuclear level densities
	WG 5	Optical model
	WG 6	Pre-compound decay
	WG 7	Fission theory
	WG 8	Nuclear model computer codes

Thursday, 11 December, evening

Session 7 Final plenary (Chairman: J.J. Schmidt)

Plenary discussion and approval of the working group reports.

Annex IV

List of participants

Benzi, V.	Italy	Centro di Calcolo del C.N.E.N, Bologna
Bergqvist, I.	Sweden	Tekniska Hoegskolan, Lund
Braga-Marcazzan, G.M. (part-time)	Italy	Centro Informazioni Studi Esperienze (CISE), Milano
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Ertek, C.	Turkey	Cekmece Nuclear Research Centre, Istanbul
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Fort, E.	France	Centre d'Etudes Nucléaires de Cadarache
Gruppelaer, H.	Netherlands	Reactor Centrum Nederland, Petten
Hadermann, J.	Switzerland	Federal Institute for Reactor Research, Wuerenlingen
Hale, G.M.	USA	Los Alamos Scientific Laboratory, Los Alamos
Igarasi, S.	Japan	Japanese Atomic Energy Research Establishment, Tokai-Mura
Jahn, H.	Fed. Rep. of Germany	Nuclear Research Centre, Karlsruhe
Janeva, N.	Bulgaria	Institute of Nuclear Research and Nuclear Energy, Sofia
Jensen, A.S.	Denmark	Institute of Physics, Aarhus
Lagrange, Ch.	France	Centre d'Etudes de Bruyeres-le-Chatel

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Visinescu, M.	Romania	Institute of Atomic Physics, Bucarest
Wiedling, T.	Sweden	AB Atomenergi, Studsvik
Wilmore, D.	UK	Atomic Energy Research Establishment, Harwell
Fonda, L. (part-time)	Italy	ICTP Trieste and Institute of Theoretical Physics, Trieste University
Rimini, A. (local secretary)	Italy	
Weber, T. (local secretary)	Italy	
Schmidt, J.J. (scientific secr.)	IAEA	Nuclear Data Section/Division of Research and Laboratories