**IAEA-190** 

# NUCLEAR THEORY IN NEUTRON NUCLEAR DATA EVALUATION Vol.1

PROCEEDINGS OF A CONSULTANTS MEETING ON THE USE OF NUCLEAR THEORY IN NEUTRON NUCLEAR DATA EVALUATION ORGANIZED BY THE IAEA NUCLEAR DATA SECTION IN CO-OPERATION WITH THE INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS, TRIESTE, AND HELD AT TRIESTE, 8–11 DECEMBER 1975



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#### Foreword

This Consultants 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.

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 1977. 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 proceedings of this meeting are published in two volumes. Volume I contains the summary report of the meeting and the review papers presented at the meeting, Volume II the contributed papers presented at the meeting.

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.

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#### 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 <u>Annex I.</u>

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

For authors, titles and numbers of review papers (RP) and contributed papers (CP) referenced in this chapter the reader is referred to the Table of Contents of Volumes I and II of these proceedings.

#### D.l. Resonance and statistical theory

#### 1. <u>General</u>

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 la, 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. <u>Statistical theory of average neutron cross sections</u>

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 (chisquared 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. <u>Statistics of cross section fluctuations</u>

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  $\gamma$ -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 El, Ml and higher multipole radiation strength functions (Brink-Axel and/or Weiss-kopf 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 sand 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  $\gamma$ -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 El-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 Ml-radiation Uhl [CP 17] uses the Weisskopf estimate.

In many cases the  $\gamma$ -ray strength function is normalized to the experimental value at the neutron binding energy. Therefore, the parameters  $\Gamma_X^{\ell=even}$  and  $\Gamma_X^{\ell=odd}$  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  $\Gamma_X$  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. <u>Uncertainty calculations</u>

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. <u>Applications</u>

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. <u>Recommendations</u>

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  $\gamma$ -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  $\gamma$ -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  $\gamma$ -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  $\gamma$ -ray strength function is introduced. A simple description of the  $\gamma$ -ray strength function is obtained by extrapolating the giant-dipole resonance strength to lower  $\gamma$ -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  $\geq 90$ . It has been observed that the model provides a good description of the  $\gamma$ -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  $\gamma$ -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  $(n, \gamma)$  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  $(n,\alpha)$ , (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 93Nb[CP 14]. A proper description of the  $\gamma$ -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 precompound 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 precompound 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  $^{235U}$ ,  $^{239}$ 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  $(^{235}U, ^{238}U, ^{239}Pu, ^{233}U)$  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. <u>Status of fission theory</u>

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 <u>a fortiori</u>, 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 common 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 semiempirical 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. <u>Status and requirements for computer codes</u>

#### 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. <u>Recommendations for further procedure</u>

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. <u>Status</u>, 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.

Title	Chapter	Chairman	Secretary	Members
General recommendations	A, B and C	M.K. Mehta	A. Prince	I. Brandus C. Ertek A. Michaudon A. Rimiri G. Ripka J.J. Schmidt
Resonance and statistical theory	Dl	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

#### 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 la Prince RP 1b Mehta plus discussion periods Session 2 Resonance and statistical theory (Chairmen: first half: L. Fonda (including capture mechanism and second half: P.A. Moldauer) nuclear level densities) 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 <u>Pre-compound decay</u> (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 <u>Fission theory</u> (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.

# List of participants

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Fonda, L. (part-time)	Italy	
Rimini, A. (local secretary)	Italy	ICTP Trieste and Institute of Theoretical Physics, Trieste Uni- versity
Weber, T. (local secretary)	Italy	
Schmidt, J.J. (scientific secr.)	IAEA	Nuclear Data Section/Division of Research and Laboratories
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

> A: Prince National Neutron Cross Section Center Brookhaven National Laboratory Upton, N. Y. 11973 USA

# Abstract:

A review of the various nuclear models used in the evaluation of neutron nuclear data for fission and fusion reactors is presented.

Computer codes embodying the principles of the relevant nuclear models are compared with each other and with experimental data.

The regions of validity and limitations of the conceptual formalisms are also included, along with the effects of the numerical procedures used in the codes themselves.

Conclusions and recommendations for future demands are outlined.

### 1.0 Introduction

The accuracies in the evaluation of neutron nuclear data necessary for the analysis of fission and fusion reactor design has attained extreme importance over the past several years.

The experimentalists with their improved techniques have been very prolific in producing neutron cross sections and related data. Nonetheless, there still exist many gaps and uncertainties that must be filled and resolved respectively.

The energy range of interest varies with the needs of the reactor specialists, however, it is evident that in general a complete knowledge of all neutron, charged particle and photon induced reactions in the energy range of thermal to 25-30 MeV is rapidly approaching.

As with the role of experimental data, many calculations based on a particular nuclear model have been sufficient in many cases and insufficient in others.

The sophistication of experimental techniques has resulted in better definition of cross sections and as a result the methods for reproducing them theoretically have required a much more elaborate interpretation.

The specific nuclear data needs for fission reactors may differ in some respects from those of fusion reactors, but in general these needs are the same in that they are primarily associated with such technological areas as nuclear heating, radiation damage, shielding, dosimetry, nuclear standards, etc. Economically the analysis that goes into the design concepts and diagnostics are very dependent upon cross sections and related data.

It is safe to say that the accuracy requirements for evaluated data, as spelled out by fast reactor physicists, have not been realized so far. The Controlled Thermonuclear Research (CTR) specialists in their acquisition of data have in many cases started with a data base developed for use in fission reactors, and in the 5-20 MeV region are finding serious gaps in required data. A typical request for data is given in <u>Table 1</u>, where the data type, energy range and accuracy for the most important reactions for the structural materials Fe, Ni and Cr in a fast breeder are presented.

In the CTR effort, since the relevent data includes cross sections, angle and energy distributions of secondary particles, it is customary to start with the same data base developed for use in fission reactors (e.g. ENDF/B, KEDAK, etc.). This is primarily due to the fact that the exact priorities and accuracies have not yet been clearly defined. However, the areas of data needs have been established and these involve such primary contributing particle reactions as  $(n,p),(n,\alpha), (n,n') (n,2n),$  etc. In some instances such rare reactions as (n,pn'), (n,n'p), may be comparable to the (n,p) reaction, thus to determine the total proton production, one must consider these tertiary reactions. So in a sense, in the 5-20 MeV region the CTR physicists are hinting at even more stringent demands than the fast reactor physicists.

A typical example of data deficiency in a structural material of importance to both fission and fusion reactors is shown in <u>Figure (1)</u>. The material is the main isotope of Cr, namely  $5^2$  Cr.

The horizontal solid bars indicate regions of sufficient measurements for defining the cross section. The dashed lines show the region where a paucity of experimental data exists and the large dots mean one or two data points. The vertical lines represent the Q value for the reactions; thus a blank space to the right of this line may be interpreted as an exposure of deficiency. Thus in order to fill this void one must resort to model calculations.

The concept of using a nuclear model today has more meaning than utility as a "stop-gap" measure. The appearance of new and improved experimental techniques have stimulated many advances in the development of theoretical nuclear models.

The purpose of this paper is to review the various methods used in analyzing nuclear reactions and to present the current nuclear models,

<u>Request for Data for Structural Materials</u>			
Material	Data Type	Energy range	Accu <b>r</b> acy requested
Cr and Cr Isotopes		l KeV - 1.0 MeV Threshold-15 MeV threshold-14 MeV 2.0 - 15 MeV 500 keV - 15 MeV	15 - 20% 25% 10 - 30% 10% 10%
Fe and Fe Isotopes		l keV - 1.0 MeV threshold-15 MeV threshold-18 MeV l keV - 16 MeV threshold-15 MeV	5 - 10% 15% 10% 5 - 20% 2 - 10%
Ni and Ni Isotopes		100 eV - 1 MeV threshold-15 MeV threshold-10 MeV 10 keV - 16 MeV threshold-15 MeV	10% 10 - 20% 5 - 15% 10% 5 - 10%

Table I

\* Compilation of Requests for Nuclear Data BNL 50444 (1975)



**REGIONS OF EXPERIMENTAL CROSS SECTION DATA FOR** 52 Cr

their range of validity, and applications. The computer codes used to typify these theoretical models will also be presented and examined in terms of intercomparisons and applications. The major emphasis will be placed on those models which have shown to be most significant in the evaluation effort. Neutron induced reactions will be of primary interest, although charged-particle reactions may be included in the general development. Consideration will be largely limited to energies ranging from the continuum to 25 MeV. Thus, the resolved and unresolved resonance regions will not be included.

### 2.0 Nuclear Reaction Model and Interpretation

Following the discovery of the gross structure in neutron cross sections  $^{(1)}$ , many experiments have provided a means for analyzing nuclear reactions in terms of a model. The physical picture underlying this model was developed primarily by Feshbach, Porter and Weisskopf.  $^{(2)}$ 

In establishing the mechanism of the interaction between nucleons and nuclei, it was customary to start with the Bohr<sup>(3)</sup> hypothesis of the formation of a compound nucleus and its subsequent decay. The energy and momentum of the incident particle was assumed to be distributed over the entire system, and the properties of the compound nucleus were independent of its formation. Thus, the subsequent decay of the compound nucleus depended only upon its over-all properties (e.g., energy and momentum).

This two-stage process of Bohr has now been replaced by a more general one due to Weisskopf, et al. (2,4) who assumed that the incident particle does not necessarily coalesce immediately with the target forming a compound nucleus, but may interact directly with one or a few of the constituents of the target.

This three-stage description is based on the following. In a first approximation the target nucleus acts upon the incident particle as a whole and may be described in the form of a potential V(r) acting on the particle, depending upon its position,  $\underline{r}$ , relative to the center of the nucleus.

The first stage of the nuclear reaction is called the "independent particle" stage, in which the particle although influenced by the nucleus (i.e., path deviated), is still distinct from the target nucleus. If the potential V(r) were just a real potential, only scattering would occur, but ascribing an imaginary part, iW(r), gives rise to an absorption. This absorption leads to the second stage of the reaction, called the Compound System.

The Compound System is more general than the Compound Nucleus concept of Bohr in that, in this state, although the particle has been removed from the entrance channel, it can still exchange its energy and momentum by collision with another nucleon, or it can initiate some surface vibration of some other collective motion. Thus the Compound System also includes the Compound nucleus, along with states caused by multiple collisions and collective excitations.

The third stage of the reaction is taken to be the breakup or decay of the Compound System into a residual nucleus and an emitted particle. If the energy exchange between the incident particle is such that it is distributed among all the constituents before breakup, then a compound nucleus is formed which has lost its "memory" about how it was formed. The decay of the compound nucleus follows certain statistical probability rules which include the possibility of a breakup into the incident particle and the original target nucleus in its ground state. This phenomenon is called compound elastic scattering, which adds coherently to the shape elastic scattering which occurs in the Independent Particle stage.

## 3.0 Optical Model

### 3.1 Gross Structure-Continuum Region

The strong fluctuations of neutron cross sections with energy are

commonly referred to as resonances. The widths of these resonances increase with energy for nuclei of intermediate mass. These widths approach or become larger than the level spacings above a few MeV. At these higher energies, therefore, the cross sections are rather smooth functions of energy. The lower energy interval is generally called the "resonance region", the upper the "continuum region".

The behavior of cross sections in the resonance region does not immediately lend itself to a description by a simple model with few parameters because of the rapid fluctuations with energy, which, moreover, depend upon the nature of the particular compound nuclear state at each resonance. The averages of the cross sections over an interval which includes many resonances, however, as shown by Feshbach, Porter, and Weisskopf (FPW), Ref. (2), are those corresponding to a new scattering problem with slowly varying amplitudes, called the "gross-structure" problem. Making the assumption that one can average over the fluctuations, FPW defined an average reflection factor  $\langle \eta_{\ell} \rangle$  which is a function of the energy of the incident particle given by

$$<\eta_{\ell}(E)> = \frac{1}{\Delta} \int_{E^{-} \mathcal{A}_{L}} \eta_{\ell}(E') dE'$$

$$(1)$$

The width of the energy interval  $\triangle$  contains many resonances but is small enough to be a smooth function of energy.

The model proposed by FPW replaced the many body problem with a onebody potential which acts upon the incident nucleon.

The potential is complex in the form

$$V = V_{o} + iW$$
(2)

where the real part represents the average potential, causing scattering, and the imaginary part the absorption, which describes the formation of the compound nucleus. The quantity  $\Pi_{\ell}$  in Equation (1) is related to the phase shift  $\delta_{\ell}$  by  $\Pi_{\ell} = e^{2i\delta_{\ell}}$ , where  $\delta_{\ell}$  is derived from the solution of the radial part of the Schrödinger equation using the potential given in (2).

### 3.2 General Formulation

The scattering and reaction processes that result from nucleonnucleus interactions have generated an enormous amount of experimental data. The variety of nuclear reactions that occur is large and attempts to explain them concisely have not been completely successful due to the properties inherent in the nuclear many body system. However, quantum mechanics has provided a means whereby a formalism for describing nuclear reactions <u>exists</u> through parameters which have a fundamental relationship with the properties of the many body system.

The foundation for this approach is manifested in the so-called Optical Model of the nucleus where it is assumed that the nucleons are scattered by nuclei in much the same way as light is scattered by a semi-transparent optical medium. The essence of the model conforms to the notion that the scattering of nucleons by complex nuclei may be described as a solution to the problem of diffraction of the nucleon wave by a particular type potential. Thus, the scattering problem is analyzed not as a many body problem, but as one of the motion of a nucleon in a certain timeindependent field produced by the target nucleus.

The nucleon's motion in this potential or, correspondingly, its wave function  $\psi(\mathbf{r})$  is determined by the Schrödinger equation

$$\frac{\pi^{2}}{2m} \nabla^{2} \Psi(\vec{r}) + E \Psi(\vec{r}) = \int V_{opt}(\vec{r},\vec{r}') \Psi(\vec{r}') d\vec{r}'$$
(3)

where the integration extends over all space.

 $V_{OPT}(\bar{r},\bar{r}')$  is a non-local potential which can in principle be selfconsistently determined from a knowledge of the individual nuclear twobody forces alone. The enormous computational difficulties involved in

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calculations, however, make such a procedure unsuitable, thus in order to simplify the solution of Equation (3), an approximate phenomenological approach is adopted whereby the non-local potential is replaced by a local, energy-dependent one.

The effective interaction experienced by an unbound nucleon when scattered in the nucleus necessarily requires that  $V_{OPT}(r,r')$  be complex, thus Equation (3) becomes

$$\frac{t^{2}}{2m} \nabla^{2} \Psi(r) + E \Psi(r) = \int V(r, r') \Psi(r') dr' + i \int W(r, r') \Psi(r') dr' + (4)$$

A local potential is defined by the equation

$$V(\vec{r},\vec{r}') = V(\vec{r})\delta(\vec{r}'\cdot\vec{r})$$
(5)

In the limit of zero range Equation (4) reduces to the usual Schrödinger equation

$$\frac{\pi^2}{2m} \nabla^2 \Psi(\bar{r}) + E \Psi(\bar{r}) = V(\bar{r}) \Psi(\bar{r})$$
(6)

where V(R) = U(R) + iW(R) corresponds to the static potential taken to be spherically symmetric. Solving this wave equation subject to the boundary conditions of incident and scattered waves gives the radial wave equation for the Lth partial wave for spin = 0 particles.

$$\frac{d^{2} U_{L}(r)}{dr^{2}} + \left\{ \frac{2m}{\pi^{2}} \left( E - V(r) \right) + \frac{L(L+i)}{r^{2}} \right\} U_{L}(r)$$
(7)

For charged particles it is necessary to add the Coulomb electrostatic field of the nucleus to the optical potential. If the particle has spin, the total wavefunction is expanded as a product of spatial and spin wavefunction, thus causing a splitting of each radial equation.

#### 3.3 Phenomenological Analysis

One of the earliest quantum-mechanical calculations of elastic scattering cross sections using a complex potential was carried out by LeLevier and Saxon.<sup>(5)</sup>

Subsequent experiments by Barschall and his colleagues, (1,6) were analyzed by Feshbach, et al. (2) who used a complex square well potential of the form

$$V = V_0 (1 + i\zeta) \quad \text{for } r < R$$
  
= 0 for r > R (8)

While this reproduced the overall features of the total cross sections for a wide range of nuclei, the square well potential resulted in too little absorption and excessive scattering cross sections at large angles.

Further investigations, <sup>(7)</sup> based on the observed properties of nuclear matter and nucleon-nucleon interactions showed that a diffuse optical potential is preferable. The shape of this diffuseness has taken many forms as seen in the Tables of Reference (8) and (9), however, the most extensively used local complex potential has the general form given by

$$V(r) = -V_R f(r, r_R, a_R) - iW_r f(r, r_r, a_r) \stackrel{\text{or}}{=} \begin{cases} i4a_P W_P \frac{d}{dr} f(r, r_P, a_P) \\ iW_S g(r, r_S, a_R) \end{cases}$$

$$+\left(\frac{K}{m_{\pi}c}\right)^{2}\frac{\vec{r}\cdot\vec{x}}{r}\left[V_{so}\frac{d}{dr}f(r,r_{so},a_{so})-iW_{so}\frac{d}{dr}f(r,r_{so},a_{so})\right] \qquad (9)$$

$$+\frac{2\vec{r}\cdot\vec{e}^{2}}{2Rc}\left(3-\frac{r^{2}}{Rc^{2}}\right)\left(r\leq R\right)a_{rd}d\frac{\vec{z}\vec{e}^{2}e^{2}}{r}\left(r>R\right)$$
where  $\frac{K}{m_{\pi}c}$  is the Compton wavelength of the  $\pi$ -meson

l = angular momentum of the incident nucleon

 $\sigma$  = spin operator

the form factor  $g(r, r_s, a_s)$  is Gaussian

$$g(r, r_{g}, a_{g}) = e_{XP} \left[ - \left( \frac{r - r_{g} A^{3}}{a_{g}} \right)^{2} \right]$$
 (10)

The remaining form factors are the so-called Woods-Saxon form

$$f(r, r_{i}, a_{i}) = \left[1 + exp\left(\frac{r - r_{i} A_{i}^{3}}{a_{i}}\right)\right]^{-1}$$
(11)

Here  $r_i$  represents the appropriate radius parameter  $r_R$ ,  $r_v$ ,  $r_D$ ,  $r_{sol}$ or  $r_{so2}$ ,  $a_i$  represents the appropriate diffuseness parameter  $a_R$ ,  $a_v$ ,  $a_D$ ,  $a_{so1}$  or  $a_{so2}$ , which are related to the target mass A by

$$R_{i} = r_{i} A^{1/3}$$
  
 $R_{c} = r_{co} A^{1/3}$ 

The first term in Equation (9) is the real central potential whose primary effect is on the shape-elastic cross section. The following three terms are the imaginary central potentials which determine the amount of absorption respectively in the nuclear volume and at the nuclear surface. They are responsible for the non-elastic processes and the compound elastic contribution to the total elastic cross section.

The next two terms are the real and imaginary parts of the spin-orbit potential. The inclusion of this potential which couples spin and orbital motion is necessitated by the fact that elastically scattered nucleons are observed to be polarized.

The final term is the Coulomb interaction potential which exists if the incident particle is charged.

As can be seen in Equation (9) the general potential has 16 adjustable parameters which is so complicated that little meaning can be attached to any calculations resulting from its use. Experience has shown<sup>(10)</sup> that it is sufficient to describe the imaginary potential with a volume or surface peaked term or a combination of the two, however the surface peaked term should be either the derivative Saxon-Woods or the Gaussian form, not both.

It has also been established that the imaginary spin orbit potential is not needed to explain polarization data except possibly, in the higher energy range. Taking these observations into consideration yields a potential of the form

$$V(r) = -V_{R} f(r, r_{R}, a_{R}) - i W_{v} f(r, r_{v}, a_{v}) + i + a_{D} W_{D} \frac{d}{dr} f(r, r_{D}, a_{D})$$

$$+ \left(\frac{t}{m_{\pi}c}\right)^{2} \frac{\overline{\sigma} \cdot \overline{R}}{r} \left\{ V_{so} \frac{d}{dr} f(r, r_{soll}, a_{soll}) \right\}$$
(12)

for neutrons.

Assuming  $r_v = r_R$  and  $a_v = a_R$  in Equation (12) yields a potential with 10 adjustable parameters  $V_R$ ,  $r_R$ ,  $a_R$ ,  $W_V$ ,  $W_D$ ,  $a_D$ ,  $r_D$ ,  $V_{SO}$ ,  $r_{SO1}$ ,  $a_{SO1}$ . Further reduction can be obtained by letting the radial parameters for the spin-orbit term be equal to those of the real central potential. At any rate, the number of parameters used in the optical model potential makes the avoidance of any ambiguity difficult.

Also one should keep in mind that the potential given by Equation (9) is only an approximation to the optical model potential given in Equation (3) and may fail to describe the experimental cross section data for any number of reasons.

Nonetheless, it has been shown that when various restrictions are applied, an optimum set of parameters may be derived which allow adequate analysis of elastic scattering of nucleons.

# 3.4 Methods of Solution

## 3.4.1 Spherical Potentials

Using the phenomenological potential V(r) the computational methods for solving the radial wave equations must be carried out numerically with the aid of computers. Many automatic techniques have been developed in the form of computer programs, for calculating the differential elastic scattering cross sections  $\sigma(\theta)$ , the total reaction cross section  $\sigma_{\rm R}$  and the polarization P( $\theta$ ), for particles of spin 0, 1/2 and 1.

These calculations involve the numerical integration of the radial Schrödinger equations for the effective partial waves. The scattering complex phase shifts are obtained by matching the logarithmic derivatives of the numerically obtained wave functions to those of the Coulomb or spherical Bessel functions.

The scattering phase shifts  $\delta_{\ell}^{\pm}$  are related to the coefficients of the outgoing waves by  $\eta_{\ell}^{(j)} = \exp(i\delta_{\ell}^{(j)})$ . For neutrons the shape elastic scattering cross section is given by

$$\sigma_{se} = \pi \chi^{2} \sum_{k=0}^{\infty} \left\{ (k+i) \left| 1 - n_{e}^{(k+i)} \right|^{2} + \lambda \left| 1 - n_{e}^{(k-i)} \right|^{2} \right\}$$
(13)

and the differential shape elastic cross section is given by

$$\frac{d\sigma_{se}}{d-r} = \left\{ \left| A(\theta) \right|^2 + \left| B(\theta) \right|^2 \right\}$$
(14)

where A( $\theta$ ) and B( $\theta$ ) are expressed in terms of the Legendre function P<sub>l</sub> ( $\cos\theta$ ) and its associated function P<sub>l</sub><sup>1</sup>( $\cos\theta$ ).

The cross section for compound nucleus formation which includes the compound elastic component is expressed as

$$\delta_{e} = \pi \chi^{2} \sum_{\ell=0}^{\infty} \left\{ (\chi_{+1}) T_{e}^{(\chi_{+1})} + \chi T_{e}^{(\chi_{-1})} \right\}$$
(15)

where  $T_{\ell}^{(j)}$  are the transmission coefficients which are related to  $\eta_{\ell}^{(j)}$  by

$$T_{g}^{(j)} = 1 - |\eta_{g}^{(j)}|^{2}$$
(16)

For protons or charged particles [e.g.  $_2\text{He}^4$  and  $_1\text{H}^2$ ] the potential now must include the Coulomb interaction and the various quantities used in describing the cross sections and scattering must now consider the phase shift of the Coulomb scattering.

# 3.4.2 Non-Spherical Potentials

The large amount of experimental data accumulated in recent years has demonstrated that many important properties of nuclei in regions 90 < N < 112

and 88<Z and Zel3 may be correlated by the strong-coupling unified model which assumes that various nuclei and their related average potential fields possess large equilibrium deformations. These large deformations have been shown to exert strong influence on the scattering and absorption of neutrons when analyzed by an Optical Model. Thus any attempt to describe differential elastic scattering cross sections, penetrabilities, and all other subsequent scattering and reaction characteristics must consider the deformation.

The theory of explaining the scattering mechanism when the collective levels are directly excited by inelastic scattering without formation of a compound nucleus, and the effect of level excitation by formation and decay of a compound nucleus was first pointed out by Bohr and Mottelson. <sup>(11)</sup> The earliest application of this coupled-channel analysis was by Margolis, et al., <sup>(12)</sup> and Chase, et al., <sup>(13)</sup> who applied the idea to the calculation of low-energy neutron strength functions. Yoshida, <sup>(14)</sup> also around the same time, described elastic and inelastic scattering of higher-energy neutrons with the same concept.

With the advent of high-speed computers many people have carried out numerical calculations of scattering phenomena based on this coupledchannel analysis.

The Hamiltonian for the interacting system of deformed target nucleus and the incident particle is given as (15)

$$H = T + H_t + V(r, \theta, \varphi)$$
(17)

The optical potential  $V(r, \theta, m)$  used is assumed to be, in general, non-spherical and is defined as

$$V(r, \theta, q) = -(V+iW) \frac{1}{1 + exp\left[\frac{r-R}{a}\right]}$$

$$- 4iW_{0} \frac{e_{xp}\left(\frac{r-\bar{R}}{\bar{x}}\right)}{\left\{1 + e_{xp}\left(\frac{r-\bar{R}}{\bar{a}}\right)\right\}^{2}} - Y_{so}\left(\bar{\sigma}\cdot\bar{z}\right)\chi_{n}^{2}\frac{1}{ar} \frac{e_{xp}\left(\frac{r-\bar{R}}{\bar{a}}\right)}{\left\{1 + e_{xp}\left(\frac{r-\bar{R}}{\bar{a}}\right)\right\}^{2}} (18)$$

$$+ Y_{coul.} \left(\chi_{\pi} = \frac{\chi_{\mu}}{m_{\pi}c}\right)$$

When R and  $\overline{R}$  are assumed to be independent of angle, Eq. (18) becomes the usual optical model potential. When R and  $\overline{R}$  are made to be dependent on  $\theta$  and  $\varphi$  according to the collective nature of the target nucleus, then the following relationships hold.

If the target nucleus is spherically symmetric but is capable of vibration about that shape, then the <u>vibrational</u> deformity is described by (a, b)

$$R = R_{o} \left\{ 1 + \sum_{\lambda m} \alpha_{\lambda m} Y_{\lambda m} (\theta, \phi) \right\}$$

$$\overline{R} = \overline{R}_{o} \left\{ 1 + \sum_{\lambda m} \alpha_{\lambda m} Y_{\lambda m} (\theta, \phi) \right\}$$
(19)

However, if the nucleus is characterized by a permanently deformed surface of cylindrical symmetry (axial symmetric), then the <u>rotational</u> deformity is defined as

$$R = R_{o} \left\{ 1 + \sum_{A} \beta_{A} Y_{o} (\Theta') \right\}$$

$$\bar{R} = \bar{R}_{o} \left\{ 1 + \sum_{A} \beta_{A} Y_{o} (\Theta') \right\}$$
(20)

where  $\beta$  is the usual nuclear deformation parameter. ( $\beta > 0$  for prolate deformation;  $\beta < 0$  for oblate deformation.)

An alternative method of analyzing nuclear scattering from deformed nuclei is the distorted wave Born approximation (DWBA), and has been used very extensively, especially in those areas where the deformation  $\beta$  is small ( $\beta \approx 0.1$ ). For values of  $\beta > 0.2$  the shape for the differential inelastic scattering is adequately described, but its magnitude is greatly over emphasized.

The differential elastic cross section is even more difficult to describe for large deformation, and it is more feasible to use the conventional coupled-channels approach rather than DWBA.<sup>(15-18)</sup>

Other methods for handling inelastic scattering based on the shell model have also been investigated as a means of microscopic descriptions of collective motion in nuclei, however, they have not been used as often as an evaluation tool, so their significance cannot be commented on at this time.

J. Raynal<sup>(19)</sup> has reported the development of a "sequential iteration method for coupled equations" called ECIS, which is an approximation between DWBA and coupled channel computations.

According to Raynal, the advantage of this iterative technique over the usual coupled-channel equation methods is its ability to save on computation time. It requires a rather large storage, but the difference of computation time is so drastic that it possibly could more than compensate for this.

3.5 Determination of Model Parameters

The preceding sections have outlined the optical model formalism and have set the stage for determining its role in the evaluation of nuclear data necessary for fission and fusion applications.

There now exists a vast body of experimental data for elastic scattering of nucleons and other reactions. Yet, in spite of this abundance, there are many gaps which must be filled by model calculations.

Extensive studies have provided adequate confidence that the optical model can be employed to give precision fits in the non-fluctuating region, to elastic scattering differential cross sections, reaction cross sections, total cross sections and polarizations provided the phenomenological parameters are optimized for each nucleus at every energy.

In general it is not possible to determine the best potential for a particular set of data by direct calculation. The usual procedure is to assume a starting potential and then vary the parameters systematically, until an optimum fit to the data is achieved. When realistic potentials are used the calculations require rather complicated computer programs.

These potentials have several disadvantages in that they usually are over parametrized such that many different potentials exist that give equally good fits to the data. This potential ambiguity raises the questions regarding the physics of the situation. The following section discusses these ambiguities along with ways that have been used to either overcome them or at least minimize them.

## 3.5.1 Non-Local Potential

A method for acquiring a somewhat consistent set of parameters over a wide range of nuclides and energies has been introduced, in which the local potential is replaced by a non-local potential. This method for computing the various cross sections from an Optical Model code was first introduced by Perey and Buck.<sup>(20)</sup> Whereas the optical model potential given earlier is both energy dependent and local, i.e.,

$$V(\overline{r'}, \overline{r}) = V(r) \ \delta(\overline{r'} - \overline{r}), \qquad (21)$$

the optical potential of Perey and Buck is energy independent and non-local.

The interpretation is that the potential acting on a particle centered at position  $\bar{r}$  does not only depend on  $\bar{r}$ , but also on the value of the wave function over all space and thus takes into account the finite size of the incident particle and the dispersive properties of the nucleus. The non-locality enters through the application of a potential term which leads to an integro-differential Schrödinger equation

$$\left\{\frac{\hbar^{2}}{2m}\nabla^{2}+E\right\}\Psi(\vec{r})=\left\{V_{SR}\ S(r)\,\vec{\chi}\cdot\vec{e}\right\}\Psi(\vec{r})\ +\ \int V(\vec{r},\vec{r}\cdot)\ \Psi(\vec{r}\cdot)\,d\vec{r}\cdot$$
(22)

where  $V(\vec{r},\vec{r'})$  is the non-local potential. This potential may be represented phenomenologically by

$$V(\overline{r},\overline{r}) = V\left\{ \frac{1}{2} (\overline{r} + \overline{r}) \right\} \frac{1}{\pi^{3} \mathcal{L} \mathcal{G}^{3}} e_{\chi p} \left\{ - \left( \frac{\overline{r} - \overline{r}}{\mathcal{G}} \right)^{L} \right\}$$
(23)

where  $\beta$  is the range of the non-locality.

As  $\beta$  approaches zero the non-local potential tends toward a local potential. The forms of the shape factors are analogous to those of the local potential. Perey and Buck<sup>(20)</sup> found that the scattering cross sections given by the non-local potential could also be adequately fitted by a local potential, and vice versa, which led to a single non-local potential that produced satisfactory agreement over an energy range of 1 to 25 MeV. The relation between the equivalent local and non-local potentials may be expressed as

$$V_{L}(r) = V_{N}(r) \exp \left\{ -\frac{m\beta^{2}}{25^{2}} (E - V_{L}(r)) \right\}$$
 (24)

Wilmore and Hodgson, <sup>(21)</sup> following the work of Perey and Buck, <sup>(20)</sup> produced an analytical set of equivalent local potentials based on energy and mass number which yielded very good cross section results from 1 to 15 MeV for medium and heavy nuclei. This method of using an equivalent non-local potential has also been used by Lane, et al., <sup>(22)</sup> and Engelbrecht and Fiedeldey. <sup>(23)</sup>

### 3.5.2 Folding Model

The use of the equivalent-local potential while yielding good fits to a wide range of nuclei, still does not quite overcome the ambiguities derived from the inter-relationship between various potential parameters.

One method for overcoming this difficulty was offered by Feshbach<sup>(8)</sup> who suggested using a volume integral of the potential

$$J = \int V(r) dr \tag{25}$$

which is a better measure of the potential strength. This is due to the inclusion of the contributions from the well depths along with the geometry. Such an approach was made by Greenlees, et al.  $(^{24},^{25})$  who analyzed the real part of the optical model potential in terms of an overlap integral of the nuclear density distribution with an assumed nucleon-nucleon interaction.

This folding procedure manifested itself in what Greenlees, et al. (24, 25) called the Reformulated Optical Model (ROM).

Greenlees and his collaborators expressed the optical model potential

in the following form

$$U_{opt}(r) = -VI(r)/I(0) - W_{v}f(r, r_{2}, q_{2}) + W_{0}a_{a_{I}}\frac{d}{dr}f(r, r_{2}, q_{I})$$
(26)  
+  $V_{s}\lambda^{v}/r\frac{d}{dr}f_{m}(r)\vec{s}\cdot\vec{x} + V_{c}(r)$ 

where  $V_{c}(r)$  is the potential due to a uniformly charge sphere of radius  $R_c = r_c A^{1/3}$ ,  $f(r, r_1, a_1)$  is a Woods-Saxon form factor, and  $f_m(r)$  is related to the matter distribution,

$$f_{m}(r) = e_{m}(r) / e_{m}(o) = \left\{ 1 + e_{x,p} \left( \frac{r - R_{m}}{a_{m}} \right) \right\}^{-1}$$
(27)

given by

$$f_{I}(r) = \left\{ i + e \times p \left( \frac{r - R_{I}}{a_{I}} \right) \right\}$$

The folded potential I(r) is represented as

$$\mathbf{I}(r) = \int P_m(\bar{r}') U_d(1\bar{r} - \bar{r}') d^3r' + \int P_ne(\bar{r}') U_n(1\bar{r} - \bar{r}') d^3r' \qquad (28)$$
$$P_m(\bar{r}) = P_n(r) + V_n(r)$$

where  $\rho_{p}, \ \rho_{n}, \ \text{and} \ \rho_{m}$  are the proton, neutron, and matter distributions of the target nucleus.

$$(\gamma_{c}(\cdot))=(\gamma_{c}(\cdot)-(\gamma_{c}))$$
 is the neutron excess distribution and  $\gamma = +/$  for protons, -1 for neutrons.

A Yukawa form was chosen to describe the central potential

$$U_{\rm d}(\mathbf{r}) = \exp(-\mathbf{u}\mathbf{r})/_{\rm ur} \tag{29}$$

As a first approximation, it was assumed that the protons and neutrons had the same density distribution, such that

$$\rho_{P}(r) = \frac{2}{4} \rho_{m}(r)$$

$$\rho_{n}(r) = \frac{N}{4} \rho_{m}(r)$$

$$U_{2}(r) = \xi U_{d}(r)$$
(30)
(5) being a constant)

( $\xi$  being a constant)

and

Thus, the real central potential given by Eq. (26) may now be expressed as

$$VI(r) = U_{RS}(r) = \int (1 + \varepsilon \xi) \rho_n(\bar{r}) V_d |\bar{r} - \bar{r}| d^3 r' \qquad (31)$$

$$(N - Z)/A.$$

where  $\varepsilon = (N - Z)/A$ ,

In order to overcome the various ambiguities inherent in multiparameter search procedure, Greenlees, et al. following Feshbach<sup>(8)</sup> derived a volume integral for this real part of the potential. The volume integral of  $U_{RS}$  is designated by  $J_{RS}$  and is related to  $J_d$ , the volume integral of the two-body interaction by

$$-\int U_{RS}dF = \overline{J}_{RS} = A \overline{J}_{d} \left( 1 + \frac{N-\overline{2}}{A} \overline{\xi} \right)$$
(32)

or

$$\frac{J_{RS}}{A} = J_{J} + \xi J_{J} \left(\frac{N-2}{A}\right)$$
(33)

The strength  $V_{RS}$  of the central potential  $U_{RS}$  was treated as a parameter and the radial parameters for the spin-orbit potential were taken to be the same as the central potential. This reduced the number of parameters from the conventional ten to eight.

The model was applied to proton elastic scattering data at 14.5, 30.3, and 40.0 MeV  $^{(24)}$  and neutron scattering at 14.5 MeV  $^{(25)}$  and yields results comparable to the conventional phenomenological analyses, although the number of adjustable parameters have been decreased by two.

Further investigation, (26-28) using a Gaussian effective interaction  $u_d(r) = exp(-kr^2)$  in Eq. (26) reduced the number of adjustable parameters to six (V,  $W_v$ ,  $W_D$ ,  $V_S$ ,  $r_1$  and  $a_1$ ).

The reasonable success of the folding model concept, while not fully tested at lower energies, e.g., E < 10 MeV, does provide a means for relating some of the nuclear structure characteristics such as the range of the two-body forces and the geometrical properties of the nucleus to the scattering data by means of the optical model. Thus, the folding integral given by Eq. (32) constitutes a rather meaningful approach to parametrizing the optical model.

Further details concerning this approach not only for neutrons and protons, but also in the analysis of the scattering of composite projectiles, may be found in Jackson  $\binom{29}{30}$  and Hodgson.  $\binom{30}{30}$ 

# 3.5.3 Minimization Technique

In order to determine an optimum set of parameters for the calculation of cross sections, the usual procedure is to carry out a least squares fit and minimizing the quantity  $\chi^2$  given by

$$\begin{aligned} \chi^{2} &= \left\{ W_{t} \left( \frac{\sigma_{t}^{\operatorname{cal}} - \sigma_{t}^{\operatorname{exp}}}{\Delta \sigma_{t}} \right)^{2} + W_{el} \left( \frac{\sigma_{el}^{\operatorname{cal}} - \sigma_{el}^{\operatorname{exp}}}{\Delta \sigma_{el}} \right)^{2} + W_{1} \left( \frac{\sigma_{1}^{\operatorname{cal}} - \sigma_{1}^{\operatorname{exp}}}{\Delta \sigma_{1}} \right)^{2} \\ &+ W_{ela} \sum_{\theta} \left( \frac{\frac{d\sigma_{el}^{\operatorname{cal}}(\theta)}{d\Omega} - \frac{d\sigma_{el}^{\operatorname{exp}}(\theta)}{d\Omega}}{\Delta \frac{d\sigma_{el}(\theta)}{d\Omega}} \right)^{2} + W_{1a} \sum_{\theta} \left( \frac{\frac{d\sigma_{1}^{\operatorname{cal}}(\theta)}{d\Omega} - \frac{d\sigma_{1}^{\operatorname{exp}}(\theta)}{d\Omega}}{\Delta \frac{d\sigma_{1}(\theta)}{d\Omega}} \right)^{2} \right) \\ &/ (W_{t} + W_{el} + W_{1} + \sum_{\theta} W_{ela} + \sum_{\theta} W_{1a}), \end{aligned}$$
(34)

where  $\sigma_{\rm T}$ ,  $\sigma_{\rm e1}$ ,  $\sigma_{\rm 1}$  are the total, elastic and inelastic cross sections, and  $\underline{d\sigma(\theta)}$  the corresponding differential scattering cross sections.  $\Delta \sigma$  is the error and Wi the weighting factors. Most analyses consider only the differential scattering cross sections. When polarization data exist, they are also taken into account by

$$x_{po1}^{2} = \sum \left[ \frac{P(\theta)^{ca1} - P(\theta)^{exp}}{\Delta P(\theta)^{exp}} \right]^{2}$$
(35)

The search is made on any number of the parameters given in Eq. (12).

Often when one is attempting to define a "global" set of parameters the data for one type of target nucleus at various energies will produce a set of parameters which exhibit wide fluctuations. This is also true for different target nuclei at a single energy. The usual procedure is to hold one set constant or limit the range and then calculate optimum values for those remaining.

The number of variable parameters in Eq. (12) can be reduced by recognizing that  $V_R r_R^n$  = constant where  $n \approx 2$  will produce equivalent fits for different values of  $V_R$  and  $r_R$  (the same holds true for  $W_D a_D^m$  = constant where  $m \approx 0.8$ ).

Thus, by holding  $r_R$  and  $a_D$  constant only  $V_R$ ,  $a_R$ ,  $W_D$ ,  $r_D$ , need be varied, where it is assumed that  $r_D = r_{S0} = r_R$  and  $a_D = a_{S0} = a_R$ . In the case of a coupled-channel calculation, the deformation  $\beta$  may also be varied.

It should be mentioned that the  $\chi^2$  method is merely a selective procedure with no absolute significance and comparing values of  $\chi^2$ with different experiments has no real meaning. This non-uniqueness manifests itself usually in attempts to calculate the inelastic cross section. While a set of parameters from a  $\chi^2$  test might produce excellent agreement with the elastic cross section, it might fail totally in reproducing an acceptable value for the inelastic.

A typical example of the  $\chi^2$  fitting procedure was carried out for both neutrons and protons by Becchetti and Greenlees<sup>(31)</sup> to determine an optimum set of nucleon-nucleus OM parameters for A > 40 and for energies less than 50 MeV.

The criterion function F of the theoretical fit was taken to be

$$F = \sum_{n=1}^{n_{max}} \left\{ \frac{\chi^2}{N_{\sigma(0)}} + \frac{\chi^2}{N_{p(0)}} + \chi^2_{\sigma_R} \right\}$$
(36)

where:

 $\chi^2/N_{\sigma(\theta)}$  = the  $\chi^2$  per point value of the differential cross sections  $\sigma(\theta)$  for the nth data set

 $\chi^2/N_{P(\theta)}$  = the  $\chi^2$  per point value of the polarization data P(A) for the nth data set;

and

 $\chi^2_{\sigma R}$  = the  $\chi^2$  value of the reaction (protons) or total (neutrons) cross section for the nth data set.

A quantity  $\chi^2/N$  is defined by

$$\frac{1}{N} = \sum_{N} \left\{ \frac{g^{\circ n}(\theta) - g^{\circ bs}(\theta)}{\Delta g^{\circ bs}(\theta)} \right\}^{c}$$
(37)

where  $g^{OM}(\theta)$ ,  $g^{obs}(\theta)$ , and  $\Delta g^{obs}(\theta)$  are the OM prediction,

the experimental value and the error in  $g(\theta)$ , where  $g(\theta)$  was taken to be  $\sigma(\theta)$ , (differential elastic scattering),  $\sigma_R$  (reaction cross section),  $\sigma_m$  (total cross section) and P( $\theta$ ) (polarization).

Further details of the fits may be found in Reference (31).

Many other systematic studies have also been made to produce a "best set" of optical model parameters. The most complete compilation of these sets have been tabulated by Perey and Perey.<sup>(32)</sup>

In addition, Aver'yanov and Purtseladze<sup>(33)</sup> have analyzed experimental data on neutrons and protons having energies ranging from 2.5 to 96 MeV, and have described a set of parameters for nuclei ranging from C to Pb.

Englebrecht and Fiedeldey  $(^{23})$  have also proposed a set of OM parameters for energies between 1 and 100 MeV.

In another attempt to avoid the ambiguity of the real and imaginary potentials, the mean values for the volume integrals of U and W were determined, using the least squares procedure for a range of nuclei of mass 20 to 210 by Holmqvist and Wiedling.<sup>(34)</sup> These generalized OM potentials provided fits that were almost as good as those from a five parameter best fit set.

### 4.0 Statistical Model

## 4,1 Semi-Classical

The statistical theory of nuclear reactions is based on the compound nucleus picture of Bohr,<sup>(3)</sup> and has been used for many years to describe in a quantitative manner a large segment of nuclear data. In the Bohr assumption it is hypothesized that the incoming particle shares its energy with the other constituants of the nucleus, thus creating an equilibrium system called the compound nucleus. This configuration "forgets" how it was formed, and may decay in many different ways.

This analogy with a classical thermodynamic system leads to an expression for the cross section of a nuclear reaction:

$$X(a,b)Y$$
 (38)

of the form

$$\sigma(\mathbf{a},\mathbf{b}) = \sigma_{\mathbf{a}}(\mathbf{a})\mathbf{P}_{\mathbf{a}}(\mathbf{b}) \tag{39}$$

where  $\sigma_c(a)$  is the cross section for formation of the compound nucleus from incident particle a on target X and  $P_c(b)$  is the probability that the compound system upon being formed will decay by emission of particle b. This concept formed the basis of the "evaporation" model developed by Ewing and Weisskopf<sup>(35)</sup> who derived a suitable form of  $P_c(b)$  based on the principle of detailed balance.

The probability per unit time of the compound nucleus decaying into an open channel leading to the emission of a particle  $\upsilon$  with energy in the interval ( $\varepsilon_{\mu}$ ,  $\varepsilon_{\mu}$  + d $\upsilon$ ) may be expressed as

$$P_{\nu}(\epsilon_{\nu})d\epsilon_{\nu} = g_{\nu}\left(\frac{8\pi \mathcal{M}_{\nu}\epsilon_{\nu}}{\hbar^{2}}\right)G_{\nu}^{\#}(\epsilon_{\nu})\left\{\mathcal{C}_{\nu}(E_{\nu})/\mathcal{C}_{\epsilon}(\epsilon_{\epsilon})\right\}$$
(40)

where  $g_{0}$ ,  $\mu_{0}$ ,  $\varepsilon_{0}$  are respectively, the spin weight, the reduced mass and the energy of the emitted particle.

The quantity  $\sigma_{U}^{*}(\varepsilon_{U})$  is the inverse cross section for compound nucleus formation and  $\rho_{U}(E_{U})$  and  $\rho_{c}(E_{C})$  are the level densities of the residual and compound nuclei.

The total probability of decay of the compound nucleus is given by

$$P = \sum_{\nu} P_{\nu}(\epsilon_{\nu}) d\epsilon_{\nu}$$
(41)

which is the sum of all particle probabilities.

The cross section for a particular particle emission is given by

$$\sigma(a;\epsilon_{\upsilon})d\epsilon_{\upsilon} = \sigma_{c}(a) \frac{g_{\upsilon} m_{\upsilon} \epsilon_{\upsilon} \sigma_{c}^{*}(\epsilon_{\upsilon}) \rho_{\upsilon}(\epsilon_{\upsilon}) d\epsilon_{\upsilon}}{\sum_{\upsilon} g_{\upsilon} m_{\upsilon} \int_{\varepsilon}^{\epsilon_{J}} \epsilon_{\upsilon} \sigma_{c}^{*}(\epsilon_{\upsilon}) \rho_{\upsilon}(\epsilon_{\upsilon}) d\epsilon_{\upsilon}}$$

$$(42)$$

The level density formulae used in Eq.(42) were based on a simplified Fermi gas model which in the high-energy limit may be expressed as

$$\rho(E) \propto E^{-2} e \times p \left\{ 2(aE)^{k} \right\}$$
(43)

where the constant a is related to the "nuclear temperature"  $\boldsymbol{\theta}$ .

This semi classical treatment represents the extreme application of the evaporation concept, and has been used for several decades to describe various nuclear reactions. Despite its simplicity, it has, and is still providing quick-order of magnitude estimates of many nuclear cross sections.

### 4.2 <u>General Treatment</u>

The formalism used in early evaporation theory given above suffers from two major drawbacks.

The first is due to the lack of conservation of total angular momentum and parity in the calculation of the cross sections. Thus, the description can only be applied to those transitions which lead to a continuum of final states. The other defect in the early concept concerns the reaction part of the compound-nucleus cross section which does not exhibit the giant resonance structure which is featured in the experimental data. Both of these defects are accounted for by the more general analysis.

(36) The statistical model given here is due to Wolfenstein and Hauser and Feshbach.<sup>(37)</sup>

The theory is still based on the assumption that all states of the compound nucleus which can be excited according to the conservation of energy, angular momentum and parity do take part in the reaction, however the formation and decay of the compound nucleus takes place in an incoherent manner. The result of this evaporation theory for the cross section  $\sigma < \alpha \mid \alpha' >$  integrated over all angles of the outgoing particle pairs and averaged over the resonance structure may be written

$$\sigma < \alpha_{1} \alpha' > = \pi x^{2} \sum_{J,j,R,j',e'} \left\{ (2 J+i) / (2i+i) (2 I+i) \right\}$$

$$\times \left\{ T_{\alpha'j',R'}^{J}, T_{\alpha',j,e} / \sum_{\alpha''j'',e''} T_{\alpha''j'',e''}^{J} \right\}$$

(44)

where  $\ell$  is the orbital angular momentum of the incoming particle,  $j = I + i = J - \ell$  its channel spin, while  $\ell'$  and  $j' = J - \ell$  are the corresponding values for the emitted particle. The symbols  $\alpha$  and  $\alpha'$  define a set of values characterizing the entrance and the exit channels, respectively. T stands for transmission coefficients, and are related to the optical-model phase shifts  $\delta_{\ell i \alpha}$  by

$$T_{xj,\ell}^{J} \equiv \left\{ 1 - \left| e^{-2i\delta_{\ell,d}} \right|^2 \right\}$$
(45)

The factor

$$T_{a'j'k'}^{J} / \underset{a''j''k''}{\not =} T_{a''j''k''}^{J} \propto \Gamma' / \mathcal{E} \Gamma''$$

$$(46)$$

since the transmission coefficients are proportional to the widths for decay to a given state. The sum in the denominator of (9) includes  $\Gamma'$ plus the widths of all possible decay modes competing with  $\Gamma'$ . When the spin-orbit interaction is absent the transmission coefficients involve only  $\ell$  and are independent of j and J. For incident and emerging particles of spin 1/2, j can have at most only two values  $j_{1,2} = I$  $\pm 1/2$  where I is the spin of the target nucleus in its ground state.

Under these circumstances, the cross section may be represented as a sum over  $\ell$  of the contributions from the various J values possible for each  $\ell$ . Thus, Eq. (7) now becomes:

$$\sigma \langle \alpha | \alpha' \rangle = \frac{\pi \chi^2}{\chi(2I+1)} \sum_{\mathcal{R}} \overline{T}_{\mathcal{R}\mathcal{R}} \sum_{j \in \mathcal{R}} \frac{\varepsilon^J}{(2J+1)} \sum_{\mathcal{R}''} \overline{T}_{\chi'\mathcal{R}''}} \frac{\varepsilon^J}{\chi'\mathcal{R}''} \sum_{\mathcal{R}'''} \frac{\varepsilon^J}{\chi'\mathcal{R}'''} \sum_{\mathcal{R}'''} \frac{\varepsilon^J}{\chi'\mathcal{R}'''}$$
(47)

Here  $\varepsilon_{j,\ell}^{J}$  is a quantity such that

 $\mathcal{E}_{j,\zeta}^{\mathcal{T}} \left\{ \begin{array}{l} = \\ 2, \text{ if both designations of } j \text{ are included in the range} \\ | J - 1 | \leq j \leq (J + 1), \\ 1, \text{ if one of the values of } j \text{ is included in the range} \\ | J - 1 | \leq j \leq (J + 1), \\ 0, \text{ if neither value of } j \text{ is included in the range} \\ | J - 1 | \leq j \leq (J + 1), \end{array} \right.$ 

The channel designation  $\alpha$  includes the energy of the incident particle and excitation state of the target nucleus, while  $\alpha'$  is the similar designation for the final system which includes the type and energy of the emergent particle and the state of excitation of the residual nucleus.

Eq. (47) may also be used to describe fission and capture by rewriting it in simple form as

$$\sigma_{r} = \frac{\pi \chi^{L}}{\lambda(2I+i)} \underbrace{\sum_{\ell=0}^{\infty} T_{n}(l, \epsilon)}_{f} \underbrace{\sum_{j=0}^{\infty} \varepsilon_{j,\ell}^{J}(2J+i) T_{r}(J, \epsilon)}_{r} \underbrace{\sum_{j=0}^{\infty} T_{r}(J, \epsilon)}_{r} + \underbrace{\sum_{j',\epsilon'} \varepsilon_{j,\ell}}_{j',\epsilon'} \underbrace{T_{n}(L(\epsilon'))}_{(48)}$$

(r refers to either capture or fission). The transmission coefficients for the fission and radiation channels are given by:

$$T_r(J,E) = ATT \frac{\langle \Gamma_r(J,E) \rangle}{\langle D(J,E) \rangle}$$
(49)

where  $\Gamma_r(J,E)$  is the partial width of a level of spin J formed by a neutron of energy E. D(J,E) is the spacing of levels of spin J.

For radiative capture  $T_r$  in the denominator of Eq. (48) is the total probability of radiative decay of the compound nucleus,  $T_{\gamma}$ . This radiation term  $T_{\gamma}(J,E)$  differs from the radiation transmission coefficient  $T_c(J,E)$  which is used in the numerator of Eq. (48) and gives the neutron radiative capture probability.

For fission the transmission coefficient  $T_f(J, \pi, E)$  is interpreted in terms of the Hill-Wheeler model <sup>(38)</sup> expressed as:

$$T_{f}(J, \pi, E) = \sum_{k} N(J, \pi, E - E_{fk}) P(E - E_{fk})$$
(50)

where  $N(J,\pi, E-E_{fk})$  is the number of transitional states in the saddle point of the fissioning nucleus above the  $k^{\frac{th}{t}}$  fission barrier with energy  $E_{fk}$ , and the penetrability  $P(E-E_{fk}(J,\pi))$  of the  $k^{\frac{th}{t}}$  fission barrier is given as

$$P\left\{E - E_{f_{H}}(J,\pi)\right\} = \frac{1}{1 + e_{\star}p\left\{\frac{2\pi(E_{f_{H}} - E)}{\hbar\omega}\right\}}$$
(51)

where  $\omega$  is the circular frequency of the inverted harmonic oscillator.

Recently  $^{(39)}$  a more detailed analysis of the fission process has incorporated the concept of a double hump fission barrier.  $^{(40)}$  This treatment allows the transmission coefficient to be expressed in terms of the coefficients for transmission across two peaks instead of one. Thus the fission probability is denoted by

$$\mathbf{P}_{\mathbf{F}} = \frac{\mathbf{T}_{\mathbf{A}} \mathbf{T}_{\mathbf{B}}}{\mathbf{T}_{\mathbf{A}} \mathbf{T}_{\mathbf{B}} + \mathbf{T}' (\mathbf{T}_{\mathbf{A}} + \mathbf{T}_{\mathbf{B}})}$$
(52)

where T' is the summation of all the other decay channels from the compound nucleus.  $T_A$  and  $T_B$  have the same form of Eq. (51) but different values for the barrier heights and curvature.

In Eqs. (44) and (47) the effect of fluctuations of the compound nucleuslevel widths about their average values has been ignored. However, even though the widths in different channels might be independent, the fluctuations in the numerator (Eqs.44,47) are correlated to fluctuations in the denominator. Thus, following Lane and Lynn<sup>(41)</sup> and Moldauer<sup>(42,43)</sup> the Hauser-Feshbach equation should be multiplied by a fluctuation correction factor given by

$$R_{dd'} = \left\langle \frac{\Gamma_{d}\Gamma_{d'}}{\Gamma} \right\rangle \left\langle \frac{\Gamma_{d} \times \Gamma_{a'}}{\langle \Gamma \rangle} \right\rangle$$
(53)

From a knowledge of the form of the statistical distribution of the widths, this width fluctuation factor can vary from 0.5 to unity depending on whether 2 channels or many are contributing. The effect is a decrease of the cross sections in all the reacting channels except the compound elastic which is increased since the total compound-nucleus cross section remains unchanged.

Moldauer<sup>(41,43)</sup> has also shown that a further correction must be made on the transmission coefficients when resonance interference is taken into account. The transmission coefficient is related to a parameter  $Q_{\alpha \ell}$ which varies between 0 and 1. This functional relationship is given by

$$T_{\alpha,\ell}^{R} = \frac{2}{Q_{\alpha,\ell}} \left\{ 1 - \left(1 - Q_{\alpha,\ell}^{T} - T_{\alpha,\ell}^{T}\right)^{k} \right\}$$
(54)

where  $T_{\alpha \ell}$  is the optical model transmission coefficient in Eq. (47). Using Eq. (54) the average reaction cross section can now be rewritten in a form

similar to that of Eq. (47) with correction for the width fluctuation and in which  $T_{\alpha \ell}$  is replaced by  $T_{\alpha \ell}^{R}$ . This correction is determined by the characteristics of the statistical distributions of the S-matrix elements.

Recently, a series of papers <sup>(44)to (48)</sup>have been published in which a reinterpretation of the conventional methods used in the statistical averaging techniques for the H-F theory have been advanced. Programs <sup>(46)</sup> to <sup>(48)</sup> to be used in computer experiments that produced synthetic cross sections analagous to those encountered in experimental measurements. The results were interpreted so as to determine the limitations imposed on the average values of the various quantities (e.g. matrix elements) used to generate these synthetic cross sections.

The values of these variables as obtained from the statistics were compared with those resulting from the conventional Hauser-Feshbach theory.

These numerical experiments have shown that in the presence of direct reactions, it is necessary that the fluctuation corrections to the cross sections and polarization data must be analyzed in a much more sophisticated and generalized form.

These various treatments for the reinterpretation of the Hauser-Feshbach formula differ in certain respects and are still open to question; nonetheless, the results are encouraging and upon application to a real situation the validity of the assumptions will be further tested.

The foregoing treatment of the Hauser-Feshbach method was devoted to binary reactions only, however, it can be extended to include many particle reactions.

Of special interest to dosimetry and CTR applications are the so called "rare" nuclear reactions such as  $(n,n\alpha)$ ,  $(n,\alpha n)$  or (n,np) and (n,pn) which necessitate a three-particle analysis.

This tertiary reaction is assumed to proceed as

$$\alpha + A \longrightarrow A^* \longrightarrow B^* \stackrel{i}{\longrightarrow} B$$

where  $\beta$  and  $\gamma$  are the emitted particles (n,p,d,t,He,He<sup>4</sup>) and  $\alpha$  is the particle incident on nucleus A leading to the compound nuclei A<sup>\*</sup> and B<sup>\*</sup>. Thus

$$\sigma_{\alpha,\beta\beta}^{J} = \pi \lambda_{\alpha}^{1} \frac{(2J_{+},)}{(2i_{\alpha}+1)(2I_{\alpha}+1)} T_{J_{\alpha}k_{\alpha}}(\epsilon_{\alpha})$$

$$\times \omega_{J_{\alpha}k_{\beta}I_{\beta}}^{J} (E_{0}; E_{\beta},\epsilon_{\beta}) \omega_{J_{\alpha}k_{\beta}I_{\beta}}^{I} (E_{0}; E_{\beta},\epsilon_{\gamma})$$

where  $T_{J_{\alpha}\ell_{\alpha}}^{\mathcal{J}}(\epsilon_{\alpha})$  represents the transmission coefficient of particle  $\alpha$ (e.g. a neutron) which has kinetic energy  $\epsilon_{\alpha}$ , total angular momentum  $J_{\alpha}$ , orbital angular momentum  $\ell_{\alpha}$ , and total angular momentum J that is produced jointly with the target nucleus;  $W_{J_{\beta},\ell_{\alpha}f_{\alpha}}^{\mathcal{J}}(\epsilon_{\circ}; \epsilon_{\alpha}\epsilon_{\alpha})$  is the probability of disintegration of the compound nucleus with spin J and excitation energy  $E_{\alpha}$  into a residual nucleus with spin  $I_{\beta}$  and excitation energy  $E_{\beta}$  and a particle with kinetic energy  $\epsilon_{\alpha}$ , total angular momentum  $J_{\beta}$ , and orbital angular momentum  $\ell_{\beta}$ ;  $W^{I\beta}$  is the probability of disintegration of the compound nucleus following the emission of particle  $\beta$ .

An exact calculation of the cross section given in Eq. (55) reduces to the determination of the probability of disintegration of the compound nuclei.

By assuming the lifetime of all the compound nuclei to be sufficiently long and by writing the set of detailed balancing equations for the decay series, one obtains the following equation for the three-particle reaction:

$$\begin{aligned}
\mathcal{J}_{d,\beta\gamma} &= \# \chi_{d}^{2} \underbrace{\sum_{J,J_{d'a}} (2J_{\pm 1})}_{J,J_{d'a}} T_{J_{a},\ell_{a}}(\epsilon_{d}) \\
\times \left\{ \underbrace{\sum_{J_{a},\ell_{\beta}} T_{J_{\alpha},\ell_{\alpha}}^{J}(\epsilon_{\beta})}_{J_{a'},\ell_{\alpha}} / \underbrace{\sum_{\ell_{\alpha},\ell_{\beta}} (\epsilon_{\beta})}_{\ell_{\alpha}'} \right\} \\
\times \left\{ \underbrace{\sum_{J_{a},\ell_{\beta}} T_{J_{\alpha},\ell_{\alpha}}^{J}(\epsilon_{\beta})}_{J_{\alpha},\ell_{\beta}'} / \underbrace{\sum_{\ell_{\alpha},\ell_{\alpha}} T_{J_{\alpha},\ell_{\beta}'}^{J}(\epsilon_{\beta})}_{\ell_{\alpha}',\ell_{\alpha}',\ell_{\alpha}'} \right\} \\
\times \left\{ \underbrace{\sum_{J_{a},\ell_{\beta}} T_{J_{\gamma},\ell_{\gamma}}^{J}(\epsilon_{\gamma})}_{\ell_{\gamma}'} / \underbrace{\sum_{\ell_{\alpha}'=\alpha} T_{J_{\gamma'},\ell_{\gamma'},\ell_{\gamma'}}^{J}}_{J_{\gamma'},\ell_{\gamma'},\ell_{\gamma'}'} (\epsilon_{\gamma'})}_{J_{\gamma'},\ell_{\gamma'},\ell_{\gamma'}'} \right\} (56)
\end{aligned}$$

(55)

The expressions for the n-particle reaction (n > 3) are similar.

If the density of final states is a continuous function of energy, then by summing or integrating over a definite range of energy, Eq. (44) becomes

$$\begin{aligned}
\int_{a,v} (\epsilon_{o}, \epsilon) d\epsilon &= \pi \lambda^{2} \sum_{J_{J,J,k}} \frac{(2 J + 1)}{(2 v + 1)(2 I + 1)} \\
\times \left\{ \overline{T}_{a,k}^{J}(\epsilon_{o}) \sum_{\overline{J',\ell'I'}} \overline{T}_{v_{J',k'}}^{J}(\epsilon) \rho_{v}(I, \epsilon) d\epsilon \right\} \\
&= \sum_{v_{j''I''}} \int_{d\epsilon}^{\epsilon_{o}-\rho_{v''}} \overline{T}_{v_{j'',k''}}^{J}(\epsilon) \rho_{v''}(I, \epsilon'') d\epsilon'' 
\end{aligned}$$
(57)

where the symbols  $\alpha$  and  $\alpha'$  for these incoming and outgoing channels have been replaced by a and  $\upsilon$ , respectively.

In Eq. (57) the sum in the denominator is taken over all energetically possible emitted particles  $\upsilon$ " (usually taken as n, p,d, t, He<sup>3</sup> and  $\alpha$ ) and  $\rho_{\upsilon}$  (I;E) is the level density of the residual nucleus at an excitation energy

$$\mathbf{E} = \mathbf{e}_{\mathbf{Q}} - \mathbf{e} - \mathbf{Q} \tag{58}$$

where Q is the Q value of the reaction.

It should also be noted that for simplicity the competing channels u' leading to fission or radiactive capture have been neglected.

# 4.3 Parametrization Methods

In analyzing nuclear reactions using the statistical model, one of the most important aspects is a knowledge of the level density.

Empirical information on the level density is usually obtained by analyzing

a. levels of residual nuclei from reactions such as (n,n'), (p,p'), (d,p),  $(d,\alpha)$  etc.

b. spectral shape of emitted particles

# c. slow neutron resonances and associated widths.

Some of these experimental data provide direct information on the level density while in others, they are provided indirectly. The latter method, in many instances, provides only rough estimates since the results are influenced by estimation of other nuclear quantities.

The most commonly used expressions for the level densities are due to Ericson  $^{(49)}$  and to Lang and LeCouteur.  $^{(50)}$ 

$$P(E, J) = const. (2J+1)exp(-J(J+1)) \frac{a^{1/2}exp(2Jau)}{2\sigma^{2}} \frac{a^{1/2}exp(2Jau)}{\sqrt{2}}$$
(59a)

or

$$p(\epsilon, J) = const. (2 J+1) exp \left(-\frac{J(J+1)}{2\sigma^{2}}\right) \frac{a^{\prime \prime} exp(2 \overline{\Delta U})}{\sigma \overline{\lambda}^{\prime \prime} (U+\epsilon)^{2}}$$
(59b)

which give a density of levels of spin J of a nucleus excited to an energy  $U_{\bullet}$ 

Eq. (59) is derived on the basis of the Fermi gas model of the nucleus where  $\sigma$  is the so called spin cut-off parameter and is related to the nuclear moment of inertia by

$$G^2 = \frac{2t}{\pi^2} \tag{60}$$

The nuclear temperature T is related to the nuclear thermodynamic temperature t by  $\cdot$ 

$$\frac{1}{T} = \frac{1}{t} - \frac{2}{0} \tag{61a}$$

$$\frac{1}{T} = \frac{1}{t} - \frac{2}{\upsilon + t}$$
(61b)

corresponding to either 59(a) or 59(b), respectively.

The quantity a is a characteristic parameter related to the spacing of single particle nucleon states near the top of the Fermi sea and is related to the thermodynamic temperature by

$$at^2 - t = U \tag{62}$$

where U is the effective excitation energy, given by U =  $(E + \Delta)$ ; E being the excitation energy and  $\Delta$  is a negative term representing the pairing energy of the last two protons when Z is even; of the last two neutrons when N is even; and the sum of both pairing energies for even-even A:  $\Delta = 0$  for odd-odd nuclei.

The parametrization has been carried out by several investigators (51-54) using experimental neutron resonance data.

This produced meaningful results only for a narrow range in the region where the fit was carried out. The a-parameters determined at the neutron binding energies predicted level densities which were too high at excitations near the ground state and much too large level densities for energies greater than 15 MeV.

Gilbert and Cameron (55) introduced a four-parameter formula in which they used a shifted Fermi gas formula at higher excitations which was smoothly joined to a constant temperature formula at lower energies. The fictive ground state was obtained from experimental mass differences, thus only the level density parameter, a, was left as the adjustable constant.

Carrying out a fit to the four constants in both the high and low regions produced fairly good results.

Another approach has employed the so-called "back-shifted" Fermi gas (57-59) model where the Fermi gas formula was used with both a and the ground state shift as adjustable parameters.

Dilg, et al.<sup>(60)</sup> show that using the "back-shifted" Fermi gas produces rather large negative  $\Lambda$  values for odd mass nuclei and moderately positive  $\Lambda$  values for even nuclei.

The a values while not showing any drastic odd-even effects, do show strong shell effects similar to the one parameter fits.

While the use of the four-parameter (e.g. Gilbert and Cameron) or the two-parameter (e.g. Dilg, et al.) have produced fair to excellent fits to experimental data, one must still be cognizant of the fact that the semi empirical formulas do not necessarily justify the adopted energy dependence of the level density.

Also for nuclei near closed shells the values of a and  $\triangle$  resulting from the parametrization can only be a course approximation and extrapolation beyond the range of validity can produce absurd results.
#### 5.0 Special Models

### 5.1 Pre-Equilibrium Model

There are two extremes that are encountered in the energy distribution of nucleons resulting from a nuclear reaction mechanism. The high energy end is usually described in terms of a combined direct (discrete) and compound nuclear process while the low end is explained in terms of the statistical theory where the Bohr independence hypothesis is assumed.

In between these extremes there exists a wide spectrum of intermediate stage processes characterized by what is commonly called a preequilibrium resulting from the sharing of the incoming energy with a small number of nucleons.

A model that described this pre-equilibrium condition was first proposed by Griffin. In this model a nucleon is assumed to enter the nucleus forming a one-particle (1p) zero-hole (0h) state. Upon interaction with one of the target nucleons a 2p - 1h state is formed. Further collisions create more particle-hole pairs (e.g. 3p - 2h, 5p - 4h, etc.).

The interaction of these excitons with the other nuclear particles permit various states to exist. For each group of states there is a certain number that can undergo particle emission. Therefore, a nuclear cascade is initiated which ends when statistical equilibrium is reached for a particular exciton number. The spectrum may then be calculated for each class of states.

The basic concepts necessary to analyze pre-equilibrium emission may be found in the Feshbach et al. (63) treatment of intermediate structure via statistical theory of "door-way" states. In their analysis of non-equilibrium contributions to cross sections, Grimes, et al. (64,65) have used this "door-way" concept).

The cross sections are calculated from the resonance parameters of the intermediate states rather than the level densities.

Their resulting equation for the pre-equilibrium cross section is analagous to the compound nucleus concept except the level densities and widths refer to particle-hole or the compound states and is given by  $(f_{1}) = (f_{2}) + (f_{3}) + (f_{3}$ 

$$\sigma_{\alpha\beta}(E)dE = \frac{(25+1)m\sigma_{\alpha}abs.(E_0)\sigma_{\beta}inv.(E)Ep'(E_0-E)}{\pi^2 t^2} \qquad (63)$$

where m and S are the mass and spin of the emitted particle;  $\rho'(E_o-E)$ is the level density of states in the residual nucleus which are available to the emission from an intermediate state; and  $\rho_{int}(E^*)$  is the density of intermediate states in the compound nucleus at excitation energy E\*. The quantities  $\sigma_{\alpha,abs}$  and  $\sigma_{\beta inv}$  are the absorption cross section for particle $\alpha$  and the inverse cross section for the formation of the door-way state by particle  $\beta$ .  $\Gamma_{int}$  is the average door-way width. To obtain the total cross section, one must add Equation (63) to the conventional equilibrium (standard evaporation) result.

An excellent review of the various models used in describing preequilibrium phenomena involving neutrons may be found in References (66) and (67).

#### 5.2 Intermediate Structure Model

Following Feshbach's and his collaborators suggestion that doorway states having a finite lifetime could give rise to intermediate structure observed in neutron total cross section, several investigators (68) have used this concept to interpret these characteristic peaks.

Beres and his collaborators have concentrated their efforts on the imaginary potential used to calculate the absorption cross section by considering a non-local energy dependent potential based on the "doorway" model with particle-vibration coupling. Other investigators (see References in Ref. 68) have also carried out similar calculations for the imaginary potential. The results of these analyses are rather encouraging; however, in most instances they have only been applied to special cases (e.g. magic nuclei -  $Ca^{40}$ ,  $Pb^{208}$ , etc.) and attempts thus far to extend them to other regions have not been as successful.

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#### 6.0 Model Codes and Their Application

In the previous section an attempt was made to review the various models that are commonly used in the evaluation effort. These models form what one might call the "state of the art" in our concept of analyzing nuclear data for use in fission reactors and CTR applications.

Due to their complicated nature, it is necessary that sophisticated numerical techniques be adopted for obtaining results.

Thus, many computer program codes have been written which embody the ideas outlined in Sections 3, 4, and 5.

This section contains general information on several model codes, their application and comparison.

6.1 <u>General Information on Nuclear Model Codes</u>

#### ABACUS-2 (revised): E. H. Auerbach, BNL-6592 (1964)

A combined optical model and Hauser-Feshbach code capable of calculating total elastic and inelastic cross sections. Contains a multi-dimensional search procedure for obtaining best optical model potentials. Does not apply width fluctuation correction.

#### ELIESE III: S. Igarasi (JAERI-1224) 1972

Optical Model-Hauser-Feshbach calculations using non-local optical potentials, their equivalent local potentials and conventional spherical local potentials. Cross sections for excitation of discrete levels and/ or overlapping levels of residual nucleus are calculated using an extended treatment of Moldauer's Theory.

#### OPW: D. Wilmore (A.E.R.E., Harwell)

No specific details, other than it has a fast search routine for parameter fitting and will calculate equivalent local potentials from non-local parameters.

SUEZ: V. Benzi et al. (C.N.E.N., Bologna)

Square Well Potential.

#### SMOG: V. Benzi et al. (C.N.E.N., Bologna)

Many types of potentials possible.

#### ELIESE II: S. Igarasi (JAERI 1169)

"Fortran II Program for Analyses of Elastic and Inelastic Scattering Cross Sections" using optical model and Hauser-Feshbach formalism.

## ABACUS-NEARREX: No formal report. Based on ANL version of ABACUS II and NEARREX (ANL 6978).

NEARREX modifies the penetrabilities obtained in ABACUS II and computes energy averages of integrated compound elastic and inelastic scattering, with certain assumptions regarding the fission and capture widths; it also calculates fission and capture cross sections.

#### ABNER:

Reduced version of ABACUS - handles only Class I (scattering problems) and Class III (Hauser-Feshbach problems) - see BNL 6562 for further definitions - written primarily for use in PDP-10.

#### STAX II: Y. Tomita (JAERI 1191)

Similar to NEARREX except an improvement is made in handling the resonance interferences by taking into consideration the dependence of the quantity  $Q^{J\Pi}$  on the  $\frac{\Gamma}{D}$  thus assuring that  $\frac{\mathrm{don,n'}}{\mathrm{d\Omega}}$  and  $\frac{\mathrm{docE}}{\mathrm{d\Omega}}$  will never be negative.

#### INS-ELASTIC SCAT: M. Kawai (Tokyo Inst. of Technology, Japan)

Calculates differential elastic cross sections and polarization.

#### OPTICAL MODEL PARAMETER SEARCH 64: A. D. Hill (Oxford Univ.)

Automatically adjusts the optical model parameters to give best fit to experimental cross sections and polarizations. Probably a combination of an Optical Model + Hauser-Feshbach code, similar to ABACUS.

#### JUPITOR I: T. Tamura

A Coupled-Channel code that may be used for incident particles of spin 0, 1/2, or 1, interacting with vibrational or rotational nuclei. Both non-adiabatic or adiabatic approximations may be performed. Up to six states can be coupled at one time. Calculates shape elastic, total, and reaction cross sections and polarizations. (Also spin-spin interactions.) TWO PLUS (2<sup>+</sup>): C. L. Dunford (BNL), Atomics International Report NA4-SR-11706(1966)

This code is useful in analyzing even-even nuclei where it is assumed that the ground state  $(0^+)$  and the first excited level  $(2^+)$  are strongly coupled by the deformed potential. The remaining levels are treated as weak (spherical potential). The program calculates shape elastic, total, and reaction cross sections, and penetrabilities for the ground state and first excited level with deformed potential. Higher excited levels use a spherical potential. The calculation of other compound nuclear processes, e.g., compound elastic, inelastic, etc., require a modified Hauser-Feshbach analysis (e.g., NEARREX).

DUMBO: F. Fabbri and A. M. Saruis (C.N.E.N., Bologna)

Similar to Two Plus (2<sup>+</sup>). No spin-orbit coupling.

#### DANGFASI: F. Fabbri and A. M. Saruis (C.N.E.N., Bologna)

Similar to DUMBO but considers spin-orbit coupling and calculates elastic scattering phase shifts, cross sections, and polarizations for neutrons on rotational even-even nuclei by coupled channel methods. Considers the 2<sup>+</sup> rotational excited state only, but is particularly useful in analyzing low energy resonant scattering of light nuclei where both real and virtual excitations of the level are considered (See G. Pisent and A. M. Saruis, Nucl. Phys. <u>A91</u>, (1967) 561).

"JUPITØR- Karlsruhe Version": H. Rebel and G. W. Schweimer (KFK 1333)1971

A modified and improved version of Tamura's coupled-channel code JUPITØR-I. The treatment of the rotational model is improved by expanding the deformed optical model potential in terms of Legendre polynomials. Also has an automatic search option.

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## "PHASER, A FORTRAN Program to Compute Neutron Cross Sections, Polarizations, and Legendre Moments from Phase Shifts": C. J. Slavik (KAPL)

PHASER is a FORTRAN program that computes the following quantities for the scattering of neutrons from nuclei: total, elastic, and reaction cross sections, differential shape and compound elastic cross sections, differential polarizations, differential and integrated compound level inelastic cross section, compound and shape elastic Legendre moments in the center-of-mass system.

## OPTIC, "A Program for the Calculation of Nuclear Cross Sections and Legendre Moments Using the Optical Model": D. T. Goldman, et al. (KAPL)

This program calculates the shape elastic differential cross section and its Legendre moments, and the total cross sections plus resonant contributions from R-Matrix theory. It does not calculate compound elastic or inelastic and capture cross sections. It was written specifically for handling low mass nuclides (e.g., 0-16), where these latter reactions are not significant for E < 10 MeV. For energies where the resonances in the cross sections are widely separated, the program with its multi-dimensional search routine, provides an adequate set of potential well parameters.

## SCAT4, A FORTRAN Program for Elastic Scattering Analyses with the Nuclear Optical Model": M. A. Melkanoff, et al. (Univ. of Calif. Press 1961) (UCLA)

This program calculates differential shape elastic, total, and reaction cross sections, along with polarization. Does not calculate compound nucleus reactions. Spherical asymmetry assumed.

<u>CÓMNUC</u>: C. L. Dunford (BNL) Atomics International Report AIAEC-12931 (1970) unpublished

A unified code for analyzing compound nuclear reactions:  $\sigma_{n\gamma}$ ,  $\sigma_{nn'}$ ,

 $\sigma_{CE}$ ,  $\sigma_{nf}$ ,  $\sigma_{n2n}$ ,  $\sigma_{n,nf}$ . Permits a consistent calculation of the compound nucleus interactions. Employs the fluctuation and correlation corrections of NEARREX and the Q corrections of STAX II. May use transmission coefficients from spherical or non-spherical optical model calculations or can generate its own - but only for a spherical potential.

#### CASCADE: C. L. Dunford (BNL), AI-AEC-12931 (1970), unpublished

Permits the calculation of  $\gamma$ -ray or neutron cascades, i.e.  $(n, \gamma, x)$  or  $(x, n \ Y)$  e.g.  $(n, \gamma f)$  or (n, nf). The gamma ray cascade takes into consideration that particle emission is possible when  $\gamma$ -rays less than the energy of the incident particle are emitted. The neutron cascade may occur when the compound nucleus is in such a highly excited state that a neutron is emitted leaving channels other than  $\gamma$ -ray channels open.

#### JANE: J. M. Ferguson, NRDL-CP-6804, unpublished

Calculates cross sections for (n,n'), (n,p) and  $(n,\gamma)$  reactions along with angular distributions of secondary neutrons and gamma-rays from the (n,n') reaction.

The Moldauer fluctuation corrections are applied to the proton and alpha channels as well as the neutron channels.

#### BØSTAW: F. Fabbri and A. M. Saruis, RT/FI(69)30 C.N.E.N., Bologna (1969)

A program for calculating the normalized eigen functions for a nucleus bound in a Woods-Saxon well. If the potential well depth is known, it will calculate the eigen values or vice-versa. Spin orbit and Coulomb potentials are included.

#### BOUND: W. R. Smith, Trinity University

Similar to BØSTAW - useful in estimating the spin sequence of levels in a nucleus.

#### NEARREX: P. A. Moldauer, ANL 6978 (1964) unpublished

The program NEARREX takes the penetrabilities from either a spherical or deformed nucleus and corrects them accordingly to yield the various compound nucleus cross sections (e.g.  $\sigma_{n\gamma}$ ,  $\sigma_{np}$ ,  $\sigma_{nf}$ , etc.).

CINDY: E. Shelton and V. C. Rogers, see Computer Phys. Comm. 6 (1973) 99

Calculates total and differential cross sections of the type (a,b), (a,b<sub> $\gamma$ </sub>) or (a,b<sub> $\gamma\gamma$ </sub>) according to statistical compound nucleus theory of Hauser-Feshbach with or without the Moldauer modifications.

#### LIANA: W. R. Smith, Trinity University

A Hauser-Feshbach subroutine for computing compound nuclear reactions. Has Moldauer fluctuation corrections. Similar to NEARREX except gamma-ray channels are included. Requires input penetrabilities from optical model code. (e.g. ABACUS II or SCATA)

#### HFW: D. Wilmore (A.E.R.E., Harwell)

Hauser-Feshbach calculation with width fluctuation corrections, similar to NEARREX.

#### SASSI: V. Benzi et al. (C.N.E.N., Bologna)

Calculates inelastic cross sections from penetrabilities applied to Hauser-Feshbach theory.

#### HELENE: S. K. Penny (ORNL) TM-2590 unpublished

Hauser-Feshbach Moldauer method for calculating scattering and reactions proceeding through compound nucleus such as (n,n'), (n,p),  $(n,\alpha)$ , etc. Pene-trabilities calculated via optical method. Handles discrete and continuum states.

HELGA: S. K. Penny (ORNL), unpublished

Extends HELENE so as to handle a third region of excitation - pseudodiscrete region. This is felt to be important in analyzing  $\gamma$ -ray production cross sections.

TRNRX: S. C. Mathur, et al., ORO-2791-20 (1966) unpublished

A FORTRAN program for angular  $\gamma$ -ray distributions in (n,n' $\gamma$ ) reactions, using Moldauer width fluctuation correction.

<u>TRANSEC</u>: S. C. Mathur, Texas Nuclear Report, (June 1975), unpublished Calculates γ-ray angular distributions using Satchler formalism. Both of these last two codes require input data from an optical model.

JULIE: G. R. Satchler, et al., ORNL 3240 (1962), unpublished

A distorted wave theory of direct nuclear reactions. Used in conjunction with program SALLY which is also described in ORNL 3240. Computes transition amplitudes, cross sections and polarizations.

#### 6.2 Nuclear Model Codes Comparison

As seen in the preceding sections, there are many model codes available for the calculation of cross sections and other related data.

While many of these codes are based on the same model, there are many instances where significant differences arise.

These differences can have their origin in several areas. A primary source of these deviations is the numerical methods used in the programming (e.g. truncation or round-off).

Another reason arises from the conversion to another computer (e.g. IBM  $\rightarrow$  CDC).

Still others are the approximation schemes employed, the values of physical constants, etc., which often might be intermixed with the numerical procedures.

All of these possible sources are due to the proliferation of programs designed to do the same thing. Of course it is assumed that the basic formalism is applied (e.g. identical optical model potential form, level densities, etc.).

Nonetheless differences still seem to be present when calculations are carried out.

Examples of attempts to explain the cause of some of these deviations are contained in the following pages.

#### 6.2.1 Comparison of JUPITOR Calculations

About 5 years ago when it was established that one should be concerned with evaluations involving highly deformed nuclei, it was reported that several differences were observed in the use of JUPITOR (Tamura version).

In an effort to gain insight into the reasons for these anomalous results, the Nuclear Model Codes Subcommittee of CSEWG (Cross Section Evaluation Working Group-ENDF) carried out a sample calculation. The case chosen was a 0.35 MeV neutron incident upon a highly deformed nucleus namely Ho-165.

All of the calculations used the same model parameters.

The results are outlined below.

#### TableII

#### (Cross sections in barns)

<u>Calc.</u>	σ <sub>Tot.</sub>	$\sigma_{\text{Reaction}}$	<sup>O</sup> Shape Elastic	S-wave Strength Function	P-wave Strength Function
1	7.986643	3.822664	4.163979	$1.453 \times 10^{-4}$	$2.011 \times 10^{-4}$
2	7.990345	3.825876	4.164469	1.453 " "	2.015 " "
3	7.990363	3.825890	4.164473	1.453 " "	2.015 " "
4	7.986643	3.822664	4.163979	1.453 " "	2.011 " "
5	8.14142	3.88121	4.26021	1.461	2.054
6	8.01200	3.85200	4.16000	-	-

1 - JUPITOR (BNL-CDC 6600) original version I from Tamura (Univ. of Texas).

2 - JUPBO (BNL-CDC 6600) obtained from Benzi (Bologna), written originally for 7094.

3 - JUPBO (BNL-PDP-10) same as 2.

- 4 JP1 (Tamura-Univ. of Texas CDC 6600) latest version.
- 5 JUPT1 (Wong-ORNL- CDC 6600) modified version of original (ORNL-4152).

6 - JP1XR (Slavik- GE-USA- CDC 6600) modified version of original (ORNL-4152).

In addition to the above reactions the versions 2, 3 and 6 provide the integrated cross sections for the direct scattering from the  $9/2^{-}$  and  $11/2^{-}$  levels in Ho-165.

		Cross	Sections in Barns
	CDC-6600	σ <sub>direct</sub> (9/2 <sup>-</sup> ) 0.0997750	σ <sub>direct</sub> (11/2 <sup>-</sup> ) 0.0231183
JUPBO	PDP-10	0.0997744	0.0231182
JP1 XR		0.1	0.023

Judging from the values of the differential scattering it appears that the other versions of JUPITOR would yield similar values for the direct scattering. From <u>Table II</u>, only 1 and 4 are in exact agreement. The apparent differences from the others appear to be due to the modification necessary for adaptation on a different computer.

These differences ( $\sigma_{\rm T}$  < 2%;  $\sigma_{\rm R}$  < 2%;  $\sigma_{\rm SE}$  < 3%) while within the experimental accuracy of the measurement ( $\sigma_{\rm T}$  = 7.94b - R. Wagner et al. Phys. Rev. 139B(1965)29 can still be of concern when a comparison is to be made of different evaluations using the same code.

#### 6.2.2 Comparison Between Different Model Codes

Kikuchi (C.E.N. Saclay)<sup>(71,72)</sup> compared JUPITOR with the coupled channel optical model code ECIS 70 (Raynal, Saclay-unpublished) on the IBM 360. The case studied was neutron scattering on U-238 with examination of the following quantities:

- 1) C-matrix coefficients,
- 2) S- and p-wave strength functions,
- 3) Total reaction cross section,
- 4) Elastic and inelastic cross sections (integrated values),
- 5) Differential elastic and inelastic cross sections,
- 6) Polarization.

Using 5 levels as a standard (the results are almost identical for JUPITOR and ECIS 70) Kikuchi compared the above quantities at 0.1, 0.6 and 2.0 MeV. <u>Table III</u> shows the results at 0.6 MeV e.g. for 2 levels with P<sub>2</sub> expansion:  $\sigma_{reac}$  (JUPITOR) = 4.051 barns and the agreement with ECIS was -0.01%. The relative deviation in the differential cross sections and polarization is defined as

$$dev(A) = \left[ \int [\underline{A(\theta)} - \underline{A^{st}(\theta)}]^2 d\theta \right]^{1/2} [\underline{A^{st}(\theta)}]^2 d\theta$$

A = differential cross sections or polarization  $A^{st}$  = the values of the standard set  $\theta$  = scattering angle (2<sup>o</sup> - 180<sup>o</sup> with  $\Delta \theta$  = 2<sup>o</sup>)

Couplings 2 levels		2 levels	2 levels		
	Spherical Img. Pot P4	Deformed Img, Pot P2	Deformed Img. Pot P4		
σ r (mb)	4219 (+1.05%)	4051 (-0.01%)	4147 (-0.02%)		
σ t (mb)	9291 (-0.26%)	8881 (-1.87%)	8905 (-1.94%)		
$S_{0} (x10^{+4})$	1.273 (1.1%)	1.235 (-0.16%)	1.256 (0.24%)		
$\frac{S_{1}}{(x10^{+4})}$	2.019 (1.3%)	1,929 (-0.16%)	1.990 (0.14%)		
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	ERROR = VALUE $Rea1 Imag.$ $+ 0.0087 + 0.0036$ $- 0.0030 + 0.0072$ $- 0.0042 + 0.0076$ $- 0.0029 + 0.0016$ $- 0.0033 + 0.0015$ $- 0.0002 + 0.0003$ $- 0.0004 + 0.0002$	WITH JUPITOR - VALUE WITH EC Real Imag. - 0.0001 -0.0001 - 0.0003 -0.0002 + 0.0003 $< 10^{-4}$ + 0.0001 - 0.0001 + 0.0001 $< 10^{-4}$ + 0.0001 $< 10^{-4}$ + 0.0001 $< 10^{-4}$ $< 10^{-4}$ $< 10^{-4}$	IS 70 Real Imag. -0.0002 - 0.0001 +0.0002 - 0.0001 +0.0003 - 0.0001 $+0.0001 < 10^{-4}$ +0.0001 - 0.0001 $< 10^{-4} < 10^{-4}$ $< 10^{-4} < 10^{-4}$		
	0.032	0.001	0.001		
viatí elast d	0.082	0.009	0.010		
ive de Stic	0.066	0.005	0.008		
Relat inela: $(2^+)$	0.079	0.008	0.010		
Time (sec) 8.1 Memory (k bytes) 183		11.4 183	10.8 183		

Table III - Comparison of JUPITOR with ECIS70 at 0.6 MeV

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Table IV shows the difference between JUPITOR and ECIS 70 when a deformed imaginary potential is assumed instead of a spherical one. Kikuchi concludes that for the p wave strength function the greatest difference between JUPITOR and ECIS 70 occurs at 0.1 MeV (low energy). The relative errors are less than 1% with 4 levels coupling and 10% for 2 and 3 levels coupling. The reaction and total elastic scattering cross sections converge well by increasing the number of levels. However the convergence of the inelastic (direct) scattering converges much slower, with the relative error several percent with 4 levels coupling. The structure (oscillations) in the differential elastic cross sections also converge when the number of levels is increased. The differences that may occur in the polarization are somewhat more difficult to ascertain since the polarization is very small at low energies. In general the conclusion was that it is impossible to say which program is right (or wrong) from this analysis. Thus comparison with other programs becomes a necessity.

Kikuchi also investigated the differences that occur when one makes various physics assumptions in a coupled-channel calculation. These included

- a) Choice of imaginary potential (deformed/spherical)
- b) Order of Legendre expansion of the (deformed/spherical) potential
  - $(P_2 \text{ or } P_4 \text{ approximation})$
- c) Number of coupled levels

The first of these (a) is seen in <u>Table IV</u> where, while differences do occur, they are still within experimental errors. Since it is more reasonable to use a deformed imaginary potential and as the computer time is not different, the use of the deformed imaginary potential is recommended.

<u>Table V</u> shows the effect of the order of the Legendre expansion  $P_2$ ( $\lambda$ =2 only) and  $P_4$  ( $\lambda$ =2 and 4). The absolute differences in the C-matrix coefficients are less than 10<sup>-2</sup>. The relative differences in the reaction cross sections and strength functions along with the differential scattering cross sections are small and since the computer time is not significantly different the  $P_4$  expansion is recommended.

## Table IV

# Difference between deformed and spherical imaginary potential with coupling of 2 levels

1	Ener	ву		0.6 MeV $(J_{max} = 4.5)$ 2 MeV $(J_{max} = 6)$			ax = 6.5)				
Ws		Deformed (standard)		spherical		Deformed (standard)		spherical			
σr		(m	b)	4148		4175	(+0.65%)	429	6	4363	(+1.6%)
σe	L	(m	b)	4761		4957	(+4.1%)	347	1	3523	(+1.5%)
$\sigma_{in(2^+)}$ (mb)		b)	171.7		182.8 (+6.1%)		368.4		407.5	(+11%)	
S <sub>0</sub> (×10 <sup>+4</sup> )		+4)	1.256		1.279(+1.8%)		0.890		0.930(+4.4%)		
S <sub>1</sub> (×10 <sup>+4</sup> )		1	.988	2.006(+0.9%)		i.282		1.256(-2.1%)			
	$c_1^j$		Val	ue	Difference from standard		Value		Difference from standard		
1		j	n	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
0		1/	2 <sup>+</sup>	-0.0562	0.8066	-0.0276	-0.0110	0.1849	0.3658	-0.0080	+0.0238
1		1/	2	-0.2422	0.2675	-0.0117	+0.0249	-0.0722	0.5830	+0.0285	+0.0314
		3/	2	-0.2119	0.2882	-0.0212	-0.0220	-0.0199	0.5683	+0.0157	+0.0369
2		3/	2 <sup>+</sup>	<b>-0.</b> 0653	0.0583	+0.0086	+0.0034	-0.2591	0.3892*	+0.0275	-0.0131
		5/	2 <sup>+</sup>	<b>-0.</b> 0559	0.0626	+0.0079	-0.0008	-0.2504	0.3943	+0.0335	+0.0008
3		5/	2	-0.0017	0.0064	+0.0009	+0.0008	-0.0660	0.1738	-0.0223	-0.0002
		7/	2 •	<b>-0.</b> 0012	0.0100	-0.0014	<10 <sup>-4</sup>	-0.1188	0.2195	-0.0109	-0.0175
		7/	2 <sup>+</sup>					-0.0056	0.0389	+0.0088	+0.0035
		9/	2 <sup>+</sup>					-0.0101	0.0421	+0.0028	+0.0089
	tíc		do		L	0	06		L		02
dev	Elas		Ωb q			0	30		i	0.	/a
tive	• S		da			, J.	16				12
Rela	nela	(2 <sup>+</sup> )	<u>Ω</u> Ω Φ			^	50			0	10 10
<b> </b>	н		•							· · ·	
Tim	6	(sec	.)	8	.2	8.	1	1	2		0
Mem	ory	(K b	ytes	2	45	24	5	24	5	24	5

P4 expansion	P2 expansion			
4148	4052 (-2.3%)			
4761	4833 (+1.5%)			
171.7	164.9 (-4.0%)			
1.259	1.237 (-1.6%)			
1.993	1.931 (-3.1%)			
VALUE	DIFFERENCE (P2) VALUE-(P4)VALUE			
Real Imag. - 0.0562 0.8066	Real Imag. - 0.0010 + 0.0041			
- 0.2422 0.2675	- 0.0092 + 0.0013			
- 0.2119 0.2882	- 0.0092 - 0.0024			
- 0.0653 0.0583	- 0.0003 - 0.0010			
- 0.0559 0.0626	- 0.0036 - 0.0011			
- 0.0017 0.0064	- 0.0004 + 0.0001			
- 0.0012 0.0100	- 0.0003 - 0.0002			
0.010				
0.064				
O	.038			
	••••			
0	.066			
8.23	7.85			
	P4 expansion         4148         4761         171.7         1.259         1.993         VALUE         Rea1       Imag.         - 0.0562       0.8066         - 0.2422       0.2675         - 0.2119       0.2882         - 0.0653       0.0583         - 0.0559       0.0626         - 0.0017       0.0064         - 0.0012       0.0100         0       0         0       0         0       0         0       0         0       0         0       0         8.23       0			

Table V - Effect of order of Legendre Expansion (E=0.6 MeV)

The most significant differences arise in the number of levels that are coupled. These effects are shown in <u>Tables VIA</u> and <u>VIB</u>. Using 5 levels as a standard we see that very precise results are achieved when one uses 4 levels, however the computer time is rather long. Going to 3 or 2 levels we see the difference becoming greater especially in the direct inelastic scattering. At this point the investigator must consider the experimental error and choose the level structure accordingly.

Another area of examination was the optimal mesh interval and cut-off radius to be used in the numerical calculations. Since the physical assumptions play such an important role in the calculations it is rather impractical to keep the precision of the C-matrix coefficients of the order of  $10^{-3}$ . The results of Kikuchis analysis are shown in <u>Table VII</u>, where 3 levels are coupled with different mesh intervals. One sees that the computer time is highly improved with a mesh of 0.3 and 0.5 fm. Increasing the mesh interval to 0.75 fm causes the error to become very large while not improving upon the amount of computer time. Considering the errors due to the number of levels that are assumed to be coupled, the interval of 0.3 fm is recommended for 4 levels coupling and 0.5 fm for 2 or 3 levels coupling.

Kikuchi<sup>(73)</sup> has also compared various spherical optical model codes and concludes that among the codes investigated (Magali, Genoa, Kouac, ABACUS, JUPITOR ( $\beta = 0$ ) and ECIS 70 ( $\beta = 0$ )) all agree except ABACUS. Since these codes were written by different authors, one may say that they are independent of each other and the agreement establishes confidence in their use. The disagreement using ABACUS probably arises from the modifications that were necessary to convert it to the IBM 360.

C. Slavik (GE -private communication) has also made a comparison between his modified JUPITOR code (JP1XR) and 2-PLUS. Taking into consideration the very large number of options available for changing the coupling scheme employed in the calculations, Slavik attempted to find a combination that would give concurrence of agreement between JP1XR and 2-PLUS. The following options were attempted:

- (a) Real form factors vs. complex form factors.
- (b) Expansion of the coupling potential to 1st order vs. a 2nd order expansion.
- (c) Expansion of the potential in Legendre polynomials vs. a power series expansion.
- (d) Spin 0 vs. spin 1/2 for the incident particle.
- (e) Increasing or decreasing the maximum number of partial waves.
- (f) Using the adiabatic vs. the non-adiabatic approximation.
- (g) Using the vibrator vs. the rotator model.
- (h) Using negative vs. positive values of  $\beta$ .
- Increasing or decreasing the step lengths in integrating the coupled equations.

Slavik concludes that both JP1XR and 2-PLUS are correct, but due to the fact that JP1XR uses the Legendre polynomial expansion of the coupling potential and 2-PLUS uses the power series expansion, there were significant differences in the results. Thus it behooves the evaluator to keep these things in mind when he is attempting to duplicate another investigator's calculations.

The preceding investigations point out rather succinctly that when one is attempting a comparison of calculations using the same set of optical model parameters only, one cannot adequately judge the differences that may arise (e.g. JP1XR uses a different mesh size for integrating than say JUPBO). All the intricate details of the evaluation must be in hand before any conclusions can be drawn.

MeV.	
0.6	
at	
levels	
οf	
number	
of	
Effects	
1	
(a)	
)IV	
Table	

,

		2 16	evels	Spheri	cal
<sup>σ</sup> r (mb)		4148	(+0.01%)	4201	(1.4%)
<sup>σ</sup> el (mb)		4761	(-8.9%)	6737	(36.5%)
$\sigma_{in} (2^{\dagger})_{(n)}$	(du	171.7	(61.1%)		
$\sigma_{in} (4^{\dagger})_{(n)}$	(dn				
<sup>S</sup> o (x10 <sup>+4</sup> )		1.25	9 (30 %)	0.73	<b>4 (-40%)</b>
s <sub>1</sub> (x10 <sup>+4</sup> )		1,993	3 (-2.7%)	2.70	8 (32%)
•,			ERROR FROM THE S	TANDARD VALUE	
r C S	F. +	Real	Imag.	Real	Imag.
0	<b> </b> 0	- 0.0117	- 0.0090	- 0.0689	+ 0.069
	'⊣I∽	+ 0.0029	- 0.0487	+ 0.0710	+ 0.1058
+	1.010	+ 0.0302	- 0.0266	+ 0.0332	+ 0.1384
, ,	~ <sup>+</sup> ~I	+ 0.0048	+ 0.0008	+ 0.0062	+ 0.0269
7	10 <sup>+</sup> 5	+ 0.0099	+ 0.0034	+ 0.0111	- 0.0276
~ ``	2'5	+ 0.0010	- 0.0013	+ 0.0017	+ 0.0070
e	101	+ 0.0015	+ 0.0052	- 0.0057	+ 0.0052
-	-10				
1017s. 5172	b <b>ic</b>	0	105	0	.285
ivai s1s	0.	.е С	342	11	.283
	10 IS	0	569		
tañ iné lag	0.	0.0	318		
Time (sec) Memory (Ķ Byte	ss)	8.3 167	2	2 167	

	5 levels (standard)	4 levels	3 levels		
σ r (mb)	4144	4140 (-0.01%)	4137 (-0.17%)		
σ <sub>el(mb)</sub>	5225	5224 (0.00%)	5288 (+1.2%)		
$\sigma_{in(2^+)}(mb)$	106.6	103.6 (-2.8%)	122.1 (+14.5%)		
$\sigma^{+}_{in(4)(mb)}$	6.51	6.72 (3.2%)	9.18 (+41.0%)		
$s_{o} (x10^{-4})$	1.222	1.214 (0.7%)	1.247 (2.1%)		
$S_{1} (x10^{+4})$	2.047	2.052 (0.9%)	2.00 (-1.9%)		
$\begin{pmatrix} C_{\ell}^{j} & j_{+}^{\pi} \\ 0 & \underline{1} \end{pmatrix}$	VALUE Real Imag.	ERROR FROM TH Real Imag.	E STANDARD VALUE Real Imag.		
$\frac{2}{1}$	- 0.0445 0.8156	- 0.0004 - <b>0</b> .0015	+ 0.0106 - 0.0041		
$1 (\frac{1}{2})$	- 0.2451 0.3162	+ 0.0001 - 0.0009	- 0.0125 + 0.0047		
$\frac{3}{2}$	- 0.2421 0.3148	+ 0.0017 - 0.0002	- 0.0067 + 0.0031		
$\begin{pmatrix} 2\\ 3 \end{pmatrix}$	• 0.0701 0.0575	- 0.0004 - 0.0001	- 0.0005 + 0.0020		
$\begin{array}{c} 2 \\ 5 \end{array} + \overline{2}_{+} \\ 5 \end{array}$	<b>- 0.</b> 0658 0.0592	+ 0.0001 - 0.0004	- 0.0021 + 0.0006		
2( <u>5</u>	- 0.0027 0.0077	$< 10^{-4} < 10^{-4}$	- 0.0005 + 0.0002		
$3 \left\{ \frac{2}{\frac{7}{2}} \right\}$	- 0.0027 0.0104	$+ 0.0002 < 10^{-4}$	- 0.0004 - 0.0001		
iation 3 ΩP ΩP ΩP		0.002	0.020		
e der	4	0.224	0.985		
lativ elast 2 <sup>1</sup> )		0.029	0.152		
Re.		0.020	0.351		
Time (sec)	316.6	133.3	42.2		
memory (K bytes	401	10/	10/		

Table VI(b) Effects of number of levels at 0.6 MeV.

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### Table VII

Effect of mesh interval at 0.6 MeV with coupling of 3 levels  $(J_{max} = 4.5)$ 

Mes	h ir (fu	nterval n)	0	.3	0	.5	0.	75	1.0	
σr		(mb)	4137	(<0.02%)	4135	(-0.05%)	4125	(-0.3%)	4096	(-1.0%)
σ <sub>el</sub>		(mb)	5290	(+0.04%)	5298	(+0.19%)	5326	(+0.7%)	5388	(+1.4%)
σ <sub>in</sub>	(2 <sup>+</sup> )	(mb)	121.9	(-0.16%)	121.2	(-0.74%)	118.8	(-2.7%)	112.7	(-7.7%)
°in	$\sigma_{in(4^+)}$ (mb) 9.18 (<0.05%) 9.17 (-0.11%)		9.08 (-1.1%)		8.73 (-4.9%)					
$S_{0}$ (×10 <sup>+4</sup> )		1.244(-0.04%)		1.24	1(-0.30%)	1.227(-1.5%)		1.186(-4.6%)		
s <sub>1</sub>	(>	(10 <sup>+4</sup> )	2.003	03(-0.05%) 2.004(<0.05%)		2.00	3(-0.05%)	2.004	(<0,05%)	
	cj			Diffe <b>r</b> enc	ference from the value with mesh interval o					
1		j <sup>π</sup>	Real	Imag.	Real	Imag.	Real	Imag.	Real	Imag.
O	)	1/2+	<10 <sup>-4</sup>	+0.0001	+0.0004	+0.0007	+0.0024	+0.0037	+0.0002	+0.0122
1		1/2	-0.0001	-0.0001	-0.0003	+0.0004	-0.0008	+0.0010	+0.0008	+0.0019
		3/2	-0.0001	+0.0001	-0.0003	+0.0003	-0.0009	+0.0008	-0.0012	+0.0012
2		3/2+	<10 <sup>-4</sup>	<10 <sup>-4</sup>	<10 <sup>-4</sup>	<10 <sup>-4</sup>	+0.0002	-0.0002	+0.0006	-0.0007
		5/2+	<10 <sup>-4</sup>	<10 <sup>-4</sup>	<10 <sup>-4</sup>	<10 <sup>-4</sup>	+0.0003	-0.0001	+0.0010	-0.0007
3		5/2	<10 <sup>-4</sup>	<10 <sup>-4</sup>	<10 <sup>-4</sup>	<10 <sup>-4</sup>	<10 <sup>-4</sup>	<10 <sup>-4</sup>	<10 <sup>-4</sup>	<10 <sup>-4</sup>
L		7/2	<10 <sup>-4</sup>	<10 <sup>-4</sup>	+0.0001	<10 <sup>-4</sup>	+0.0001	<10 <sup>-4</sup>	+0.0001	<10 <sup>-4</sup>
۰.	tic	$\frac{d\sigma}{10}$	0.0003		0.0015		0.005		0.010	
ve de	Ela	P B	0.0014		0.006		0.019		0.047	
lati	las.	$\frac{d\sigma}{d\sigma}$	0.002		0.008		0.032		0.097	
Re1	Ine	C P	0.003		0.012		0.052		0.191	
Tin	ne	(sec.)	2	0	1	6	1	1	1	0
Memo	ry	(K bytes)	24	5	24	5	24	5	24	5

## 6.2.3 INTERCOMPARISON OF CODES FOR CALCULATING $\sigma_{nY}$

In the spring of 1974 several laboratories in the USA agreed to participate in a world-wide intercomparison study of model codes for the calculation of the radiative capture.

This idea was proposed by H. Gruppelaar (Petten) who suggested that I-127 be used as the sample case.

The main purpose of this venture was to analyze the differences in the results using various codes and not necessarily to ascertain which code produced the "best" agreement with experimental data.

Each laboratory was to use exactly the same set of parameters. e.g. optical model parameters, level density parameters, excitation energies, etc.

The response was very encouraging and the results pointed out very succinctly that certain formalisms, while using the same basic set of input data, can produce drastic differences.

Some of the results are outlined below, along with pertinent comments wherever necessary.

#### Relations between codes

The codes FISPRONE, FISPRO-5, and FISPRO-6 are derived from the code FISPRO-2.

The codes FISPRONE and FISPRO-5 are nearly identical and use the Lang and Le Couteur level density formula.

The codes FISPRO-6 and NCAP use exactly the same level density formula (Gilbert-Cameron).

In the codes CASTHY and CERBERO Moldauer theory is used.

COMNUC-3 and COMNUC-7 are modified versions of the original COMNUC-1.

The codes FISPRO-5,6 have been used to simulate the results of FISPRONE, CERBERO and NCAP as close as possible.

In <u>Table VIII</u>, the differences in the transmission coefficients range from less than 1% to approximately 9%.

#### Listing of Codes used in Tables

```
1.
     FISPRONE, CNEN, Italy
 2.
     FISPRO-5 (comparison with FISPRONE), RCN, the Netherlands
 3。
     CERBERO, CNEN, Italy
     FISPRO-6 (comparison with CERBERO), RCN, the Netherlands
 4.
 5.
    NCAP, HEDL, USA
     FISPRO-6 (comparison with NCAP), RCN, the Netherlands
 6.
 7.
     FISPRO-6 (comparison with NCAP), RCN, the Netherlands
8.
     COMNUC-3, HEDL, USA
 9。
     CASTHY, JAERI, Japan
10.
    FISINGA, CEN, France
11.
    HELGA, ORNL, USA
12.
     COMNUC-3, BNL, USA
13.
     COMNUC-3, B & W, USA
     COMNUC-7, LLL, USA
14.
```

#### Comparison of Hauser-Feshbach/Moldauer Calculations (Tables X. XI. XII, XIII)

The results of the various codes using the Hauser-Feshbach formalism with and without the Moldauer corrections are given in <u>Tables IX to XIII</u> for radiative capture and <u>Tables XIV</u> and XV for inelastic scattering and may be summarized as follows:

#### Radiative Capture

- a. E < 0.0576 MeV
  - . transmission coefficients: rather large differences (= 7%)
  - . cross sections without WFL: differences less than 3% ) WFL = width

. cross sections with WFL: differences less than 3% fluctuation correction The cross sections calculated with CASTHY and CERBERO are systematically somewhat larger than those calculated with the other codes.

- b. 0.0576 MeV < E < 0.745 MeV
  - . transmission coefficients: rather large differences for transmission coefficients of inelastic channels.

- cross sections without WFL: differences up to 10% for the highest energies.
- , cross sections without WFL: large differences up to 25%, partly due to the definition of W.

The capture cross sections calculated with CASTHY and CERBERO are systematically somewhat larger than those calculated with the other codes. The use of different formulae for the level density of the compound nucleus did not seem to be very important in this energy region; the level density of the target nucleus is discrete up to E = 0.745 MeV.

#### c. E > 0.745 MeV

- . transmission coefficients: small differences for high energies.
- . width fluctuation factor:  $\mathtt{W}\approx \mathtt{l}_{*}$
- . differences in level density formulae and parameters.

The various outcomes of the codes are difficult to compare with each other. Even if  $D_{obs}^{t} = 67.8 \text{ eV}$ , the level density of the target nucleus at low energies is not unique. Below neutron energies of about 5 MeV the level density of the composite Gilbert-Cameron formula is Maxwellian. Note the striking difference between the FISPRONE, FISPRO-5 results and the CERBERO, FISPRO-6 results.

## σ<sub>nn</sub>'

The total inelastic scattering cross sections resulting from the calculations are given in <u>Tables XIV</u> and <u>XV</u> with and without width fluctuation corrections respectively. In general the discrepancies are small at the low energies, increasing at the higher energies and in the continuum as much as 15%. This latter difference may be attributed to the fact that the n-2n competitive reaction must be considered for  $E \ge 9.15$  MeV.

In general the results point out that while the codes used essentially the same parameters, differences do occur. Part of this is due to the formalism used in the level density and whether or not one applied the width fluctuation correction.

## Table VIII

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## Transmission coefficients (optical model)

 $T_{\ell}$  (E), ( $\ell = 0, 1, 2$ )

r	E <sub>lab</sub> (MeV)	FISPRONE CNEN Italy	FISPRO-5,6 RCN Netherlands	NCAP Hanford USA	COMNUC Hanford USA	CASTHY JAERI Japan	CØMMUC3 BNL USA	Max. differ- ence
l≕O	0.001 0.010 0.1 1.0 10	0.0492 0.1477 0.3973 0.8052 0.7790	0.0506 0.1515 0.4071 0.8211 0.7765	0.0516 0.1545 0.4129 0.8221 0.7780	0.0491 0.1474 0.3979 0.8136 0.7768	0.0525 0.1570 0.4185 0.8271 0.7715	0.0491 0.1474 0.3979 0.8136 0.7768	7% 5% < 1%
L=1	0.001 0.010 0.1 1.0 10	0.00008 0.00239 0.0569 0.3914 0.6753	0.000074 0.00226 0.0538 0.3757 0.6801	0.00008 0.00232 0.0552 0.3834 0.6791	0.000074 0.00227 0.0538 0.3748 0.6795	0.000075 0.00232 0.0550 0.3830 0.6804	0.000074 0.00227 0.0538 0.3748 0.6795	3% < 1%
£=2	0.001 0.010 0.1 1.0 10	0.0 0.00001 0.00223 0.3978 0.7785	0. 0.00001 0.00233 0.4092 0.7734	0. 0.00001 0.00240 0.4152 0.7749	0. 0.000074 0.00226 0.3997 0.7747	0. 0.000080 0.00244 0.4201 0.7737	0.0 0.0000074 0.00226 0.3997 0.7747	9% < 1%

_						( · · · · · · · · · · · · · · · · · · ·				
E (MeV)	1. FISPRONE CNEN Italy	2 FISFRO-5 RCN Nether lands	3 CERBERO CNEN Italy	4 FISPRO-6 RCN Netherlands	5 NCAP Hanford USA	6,7 FISPRO-6 RCN Netherlands	9 CASTHY JAERI Japan	mean value	max. dev. Z	Comment
.001 .003 .004 .005 .007 .010 .020 .040	11.434 4.667 3.121 2.432 1.904 1.008	11.553 4.688 3.123 2.425 1.892 0.995	11.696 4.720 3.139 2.437 1.899 1.000	11.589 4.702 3.133 2.434 1.899 1.000 0.857	11.610 3.727 2.433 1.900 0.854	11.540 3.711 2.420 1.888 0.848	11.702 4.733 3.753 3.150 2.448 1.910 1.007 0.863	11.589 2.433	-1.34, +0.97 -0.53, +0.62	differences of 1 to 2%
.050 .070 .1 .3 .4 .5 .6 .7	0.764 0.555 0.400 0.177 0.139 0.109	0.756 0.551 0.398 0.176 0.137 0.109	0.758 0.552 0.400 0.177 0.139 0.114	0.760 0.556 0.403 0.182 0.162 0.145 0.140 0.120	0.549 0.396 0.170 0.140 0.131 0.125 0.105	0.547 0.395 0.172 0.150 0.132 0.127 0.108	0.766 0.559 0.406 0.184 0.165 0.148 0.143 0.143	0.553 0.139 0.112	-0.57, +0.60 -5.7, +6.5 -2.7, +8.0	differences upto 10%
.8 .9 1.0 1.5 2.0 3.0 5.0 7.0 10 12 15	0.0786 0.0394 0.0142 0.0041 0.0008 0.0003 0.	0.0784 0.0404 0.0141 0.0040 0.00078 0.00029 0.00005	0.095	0.105 0.100 0.0992 0.110 0.131 0.164 0.0739 0.6165 0.0021 0.00065 0.00008	0.090? 0.0313 0.0747 0.0541 0.0417 0.0260 0.0051 0.0010 0.0010 0.0003 0.	0.0998         0.0918           0.0803         0.0835           0.0734         0.0784           0.0556         0.679           0.0447         0.0649           0.0273         0.0648           0.0051         0.0574           0.00061         0.0174           0.00001         0.0015           0.         0.0002	0.104 0.0957 0.0901 0.0620 0.0413 0.0106 0.0183 0.0019	} not	always possible to	compar≞
level density	Lang and D <sup>t</sup> = 67 obs	Le Couteur 1.8 eV	Gilbert D <sup>t</sup> obs	-Cameron 67.8 eV	Ci'b D <sup>t</sup> = 1 obs	$\begin{array}{c} \underline{\textbf{c}} \underline{\textbf{c}} \underline{\textbf{c}} \underline{\textbf{c}} \underline{\textbf{c}} \underline{\textbf{c}} \underline{\textbf{c}} \\ \underline{\textbf{c}} \underline{\textbf{c}} \underline{\textbf{c}} \underline{\textbf{c}} \\ \underline{\textbf{c}} \underline{\textbf{c}} \underline{\textbf{c}} \underline{\textbf{c}} \\ \underline{\textbf{c}} \underline{\textbf{c}} \underline{\textbf{c}} \underline{\textbf{c}} \end{array}$	Gilbert- Cameron			

Hauser-Feshbach without width-fluctuation correction (optical model, no direct contributions, no  $(n, 2\gamma)$ )

 $(\sigma_v \text{ in } b)$ 

### Table IX

Table	Х
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Hauser-Feshbach w	<u>vith</u>	width-fluctuation	correction	(optical	model,	no	direct	contributions,	no	(n,2Y))	

 $(\sigma_{\gamma} \text{ in } b)$ 

E (MeV)	l FISPRONE CNEN Italy	2 FISPRO-5 RCN Nether lands	3 CERBERO CNEN Italy	4 FISPRO-6 RCN Nætherlands	5 NCAP Hanford USA	6,7 FISPRO-6 RCN Netherlands	8 COMNUC-3 Hanford USA	9 CASTHY JAERI Japan	mean value	max. dev. <b>X</b>	Comment
.001 .003 .004 .005 .007 .010 .030 .040	7.842 3.307 2.273 1.806 1.440 0.776	7.923 3.322 2.273 1.801 1.432 0.766	8.025 3.354 2.293 1.814 1.440 0.771	7.944 3.331 2.682 2.280 1.806 1.436 0.768	8.045 2.684 1.807 1.436 0.647	7.909 2.668 1.797 1.428 0.650	7.798 2.633 1.779 1.414 0.635	8.029 3.361 2.705 2.299 1.822 1.449 0.771 0.665	7.939 1.804 0.649	-1.22, +1.34 -1.39, +1.00	differences of 2~3%
.050 .070 .1 .3 .4 .5 .6 .7	0.588 0.449 0.343 0.179 0.146 0.118	0.580 0.436 0.334 0.175 0.143 0.117	0.584 0.435 0.331 0.167 0.134 0.112	0.582 0.438 0.338 0.181 0.167 0.151 0.147 0.128	0.436 0.331 0.172 0.158 0.140 0.130 0.113	0.431 0.331 0.172 0.156 0.139 0.134 0.115	0.409 0.320 0.153 0.137 0.120 0.115 0.0975	0.591 0.441 0.335 0.174 0.157 0.142 0.138 0.118	0.434 0.172 0.115	-5.8, +3.5 -11, +5.2 -15, +11	differences upto 25%, partly due to differences in width fluctuation factor (larger than 1 or less than 1)
.8 .9 1.0 1.5 2.0 3.0 5.0 7.0 10.0 12.0 15.0	0.0786 0.0394 0.0142 0.0041 0.0008 0.0003 0.	0.0784 0.0404 0.0141 0.0040 0.00078 0.00029 0.00005	0.095	0.105 0.100 0.0992 0.110 0.131 0.164 0.074 0.016 0.0021 0.00065 0.00008	0.0974 0.0868 0.0974 0.0521 0.0408 0.0257 0.0051 0.0010 0.00011 0.00002 0.	0.0908         0.0918           0.0803         0.0835           0.0734         0.0784           0.0556         0.0679           0.0447         0.0649           0.0273         0.0648           0.0551         0.0574           0.00061         0.0174           0.0004         0.039           0.0001         0.015           0.         0.0002	0.0869 0.0839 0.0843 0.1033 0.1233 0.1171 0.0512 0.0163 0.0045	0.103 0.094 0.0880 0.0605 0.0190	not always possible to compare		
level dnsity	Lang and D <sup>t</sup> = 67 obs	Le Couteur 7.8 eV	Gilber Dt obs	t-Cameron 67.8 eV	Gilbert-Cameron Dt =1.02 eV Dt =67.8 cbs		z.	Gilbert- Cameron			

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## Moldauer theory with width fluctuation correction

( $\sigma_{\gamma}$  in b)

E (MeV)	CERBERO CNEN Italy	CASTIIY JAERI Japan	CASTIIY JAERI Japan
.001 .003 .004 .005 .007 .010 .030 .040	8.096 3.392 2.321 1.838 1.459 0.781	8.167 3.428 2.760 2.347 1.861 1.479 0.794 0.681	8.029 3.361 2.705 2.299 1.822 1.449 0.771 0.655
.050 .070 .1 .3 .4 .5 .6 .7	0.593 0.441 0.335 0.167 0.134 0.112	0.604 0.451 0.344 0.177 0.161 0.145 0.141 0.122	0.591 0.405 0.354 0.174 0.158 0.142 0.138 0.118
.8 .9 1.0 1.5 2.0 3.0 5.0 7.0 10.0 12.0 15.0	0.095	0.106 0.0969 0.0906 0.0493 0.0155	0.103 0.0941 0.0880 0.0605 0.0190
Remarks			without inter- ference

## Table XII\*

Capture Cross Sections

		(σ <sub>nγ</sub>	, in barns)			
E(MeV)	CØMNUC3 BNL (a)	CØMNUC3 BNL (b)	CØMNUC7 LRL (a)	CØMNUC7 LRL (b)	HELGA ORNL	CØMNUCI B&W
0.001	7.797	7.797	7.934	7.934	6.937	-
0.002	4.490	4.490	-	-	-	-
0.003	3.274	3.274	-	-	-	-
0.004	2.640	2.640	2.648	2.648		-
0.005	2.240	2.240	-	-	-	-
0.007	1,780	1.780	1.784	1.784	-	-
0.01	1.410	1.410	1.419	1.419	1.173	1.409
0.02	-	-	-	-	-	0.935
0.04	0.635	0.635	0.648	0.648	-	0.628
0.05	0,560	0.560	-	-	-	-
0.06	-	-	-	-	-	0.467
0.07	0.410	0.410	0.428	0.428	-	-
0.08	-	-	-	-	-	0.356
0.1	0.320	0.320	0.324	0.324	-	0.314
0.2	0.210	0.210	0.211	0.211	0.220	0.203
0.3	0.150	0.150	0.150	0.150	-	-
0.4	0.137	0.137	0.130	0.130	-	0.129
0.5	0.120	0.120	0.112	0.112	-	-
0.6	0.115	0.115	0.106	0.106	-	0.105
0.7	0.097	0.097	0.092	0.091	-	-
0.8	-		0.080	0.079	-	0.078
0.9	0.083	0.083	0.076	0.075	-	-
1.0	0.0835	0.0835	0.074	0.073	0.041	0.070
1.5	0.098	0.098	0.075	0.074	-	-
2.0	0.107	0.107	0.074	0.074	0.037	-
2.5	-	-	0.068	0.070	-	-
3.0	0.0812	0.0257	0.0572	0.0614	-	-
4.0	0.042	0.0076	0.0317	0.0376	-	-
5.0	0.017	0.00018	0.0140	0.0186	0.014	-

\* a, b- different level assumptions were made;

E(MeV)	CØMNUC3 BNL (a)	CØMNUC3 BNL (b)	CØMNUC7 LRL (a)	CØMNUC7 LRL (b)	HELGA ORNL	CØMNUCI B&W
6.0	0.006	0.00037	0.0057	0.00858	~	-
7.0	0.002	0.00009	0.0025	0.00417	-	-
8.0	0.001	0.00004	0.00124	0.00226		-
9.0	0.00047	-	0.00089	0.00150	-	-
10.0	0.00031	-	0.0011	0.00147	0.00175	-
11.0	~	-	0.00187	0.00209	-	•
12.0	0.00049	-	0.00312	0.00132	-	-
13.0		-	0.00437	0.00437	-	-
14.0	~	-	0.00530	0.00528	-	-
15.0	0.00086	-	0.00577	0.00577	-	-

•

## Table XIII

## Direct and collective capture contribution

E (MeV)	FISPRONE CNEN Italy	FISPRO-5,6 RCN Netherlands	NCAP Hanford USA	CØMNUC3	CØMNUC7
1.0 3.0 5.0 7.0 10.0 12.0 15.0	0.00001 0.00001 0.00003 0.00008 0.00091 0.00322 0.00588	0.00001 0.00003 0.00008 0.00086 0.00309 0.00584	0.00117 0.00134 0.00167 0.00193 0.00235	0.0000008 0.000002 0.000004 0.000012 0.00013 0.00045 0.00086	0.000005 0.000012 0.000029 0.00008 0.00084 0.00305 0.00577

## Table XIV

### Total inelastic scattering cross section with

## width fluctuation correction

 $(\sigma_{nn'} \text{ in } b)$ 

E (MeV)	CERBERO CNEN Italy	CASTHY JAERI Japan	FISINGA CEN France	HELGA ORNL USA	COMNUC-3 BNL USA
0.050 0.070 0.1 0.3 0.4 0.5	0.0 0.363 0.477 0.828 1.141	0.0 0.359 0.473 0.825 0.920 1.136	0.0 0.363 0.478 0.831 0.926 1.145	0.0 0.480	0.0 0.336 0.455 0.797 0.89 1.098
0.6 0.7	1.463	1.239 1.457	1.470		1.200 1.403
0.8 0.9 1.0 1.5 2.0 3.0 5.0 7.0 10.0 12.0 15.0		1.616 1.748 1.864 2.423 2.245	1.616	1.792 2.489 2.552 2.224	1.830 2.30 1.57 2.49 2.18 1.94 1.72 1.39
Remarks	no conti- nuum calcula- tion	width fluc- tuation also in continuum	no conti- nuum calcu- lation		$\Gamma_{\gamma} = \Gamma_{\gamma}(E)$

.

## Table XV

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## Total inelastic scattering cross section without width fluctuation correction

 $(\sigma_{nn'} \text{ in } b)$ 

E (MeV)	CERBERO CNEN Italy	CASTHY JAERI Japan	FISINGA CEN France	HELGA ORNL USA
0.050	0.0	0.0	0.0	0.0
0.070	0.672	0.664	0.672	
0.1	0.865	0.855	0.865	0.862
0.3	1.329	1.322	1.332	
0.4		1.400	1.411	
0.5	1.611	1.602	1.612	
0.6		1.689	1.702	
0.7	1.880	1.871	1.888	
0.8		2.002	2.008	
0.9		2.104		
1.0	2.106	2.191		2.135
1.5				
2.0		2.534		2.489
3.0		2.674		
5.0		2.532		2.552
7.0		2.282		
10.0		2.245		2.224
12.0				
15.0				
Remarks	no conti- nuum calcula- tion		no conti- nuum calcula- tion	
## 7.0 Comparison with Experimental Data

This section is devoted to a number of representative examples showint the application of various nuclear model codes used in evaluating nuclear data.

Various reactions have been chosen to show how nuclear model codes might aid in filling the gaps that exist in experimental data and how by using various formalisms one might resolve some of the discrepancies that occur from time to time in the empirical data.

# 7.1 Coupled Channel Calculations for Vibrational Nuclei

A recent evaluation of the Cr and Ni isotopes at BNL<sup>(74)</sup> used coupledchannel calculations to determine the high energy elastic and inelastic scattering data.

<u>Figures (2) and (3)</u> show the direct and compound components for the differential inelastic scattering for the 2.369 MeV level in 52 Cr at an incident energy of 8.56 MeV, and the 1.434 and 4.34 MeV levels at 14.0 MeV.

It is obvious that the consideration of the direct component improves the fit especially for the 14.0 MeV data when the angular distribution is highly anisotropic, and is practically due entirely to the direct component.

7.2  $\sigma_{np}$  for Ni - 58

A comparison of several recent statistical model codes (all of which consider tertiary reactions) is shown in <u>Figure (4)</u>. As can be seen, all of the codes are in good agreement up to about 3.5 - 4.0 MeV, then they begin to differ, not only in magnitude, but in shape.

The reasons for these differences are many, including such things as level density formalism used; whether or not the discrete energy states of the residual nuclei exist, and if so, were the spins and parities different. Also of importance are the transmission coefficients used to obtain the inverse cross sections along with the inclusion of competitive reactions (e.g., n,pn, n,np, n,n $\alpha$ , etc.).

While all of the calculations included a pre-equilibrium contribution at the higher energies, the percentage contributions were not the same, thus, also causing slight differences.

All in all, the calculations do agree with the experimental data deviating about 20 - 30% at most.

7.3  $\sigma_{np}$  and  $\sigma_{n\alpha}$  for Cr - 52

Figure (5) shows the calculations of  $\sigma_{np}$  and  $\sigma_{n\alpha}$  for <sup>52</sup>Cr. The curves show the results of codes THRESH and HAUPT. The (n-p) THRESH calculations were normalized to the 14 MeV data of Kenna and Harrison, <sup>(75)</sup> while the  $(n-\alpha)$  THRESH were normalized to the single experimental data point of Dolya, et al. <sup>(76)</sup>

The HAUPT calculations were carried out without any normalization. The n-p reaction using HAUPT deviates rather strongly from the experimental data of Kern, et al., (77) for energies greater than 17 MeV. However, according to Kern, et al., (77) their experimental data might be too large due to contamination problems.

This fall off of the HAUPT calculations still might be too drastic due to the fact that direct contributions have not been taken into consideration.

# 7.4 Fission Cross Section for U-239

Figure (6) shows the recent calculation for the fission cross section of  $^{239}$ U, carried out by D. Gardner $^{(78)}$  using CØMNU-7. A comparison with an older calculation, and that of Jary $^{(79)}$  is also shown along with the inferred experimental results of Cramer and Britt. $^{(80)}$ 

The difference between the old and new calculation was an increase in the number of open channels (thereby decreasing the compound elastic cross

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section); and an improved level density approximation for  $^{240}$ U along with a slight decrease in the height at the lowest fission barrier.

As can be seen, these changes seem to improve the agreement with those of  $Jary^{(79)}$  and Cramer and Britt. (80)

# 7.5 Inelastic Scattering for U-238

One of the most important reaction cross sections for  $U^{238}$  are the inelastic excitation for the first two excited levels at 0.045 and 0.148 MeV.

Early measurements by Barnard (81,82) have been questioned and the consensus is that around 0.5 MeV, the inelastic cross section for the 0.045 MeV level is too high.

Another discrepancy exists for both of the levels at energies greater than 1.3 MeV. Where earlier calculations assumed only compound inelastic scattering, and used the statistical model to estimate the inelastic cross section, recent measurements at Lowell Tech. <sup>(39)</sup> and at ANL <sup>(83,84)</sup>have shown that a direct component must also be considered.

<u>Figures (7) and (8)</u> show the results of calculations using JUPITOR for the direct component and COMNUC (with transmission coefficients from JUPITOR) for the statistical part.

Also shown are the calculations reported by  $Jary^{(85)}$  at the recent Kiev conference.

# 7.6 Total Cross Section for Pu-239

In Figure (9) a JUPITOR calculation<sup>(86)</sup> of the total cross section for Pu<sup>239</sup> is compared with experimental data. It is in excellent agreement with all the experimental data except that of Cabe<sup>(87)</sup> where it is about 5% too low.

#### 7.7 Fission Cross Section for Pu-239

<u>Figures (10) and (11)</u> show the calculation  $(^{86})$  of the fission cross section of Pu<sup>239</sup> carried out using the CØMNUC code. It is clearly seen

that the calculational results are, in general, within 0.1 to 0.2 barns of the recommended values and well within the accuracy of the experimental data which shows a wide dispersion over the entire energy range.

7.8 Scattering Cross Section for Pu-239

<u>Figures (12 - 15)</u> are included to point out the implications involved in evaluating experimental scattering data.

The lowest lying level of Pu-239 is at 8 keV and practically all differential scattering is contaminated with a contribution from this level.

The first set of these, <u>Figure (12)</u>, shows the experimental data of Cavanagh<sup>(88)</sup>, Knitter and Coppola<sup>(89)</sup>, and Cranberg. <sup>(90)</sup> According to Knitter and Coppola<sup>(89)</sup>, their measured values included contributions from not only the 8 keV level but also the next two higher levels at 57 and 76 keV. Thus, to compare the calculations with their experimental data, the contributions from both compound and direct inelastic scattering must be included. <sup>(86)</sup>

At the higher energies, (E > 1.0 MeV) the direct contributions of the first two levels must definitely be considered as seen in <u>Figures (13)</u> to (15).

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## 8.0 <u>Conclusions and Recommendations</u>

In the preceding pages, an attempt has been made to give a <u>status</u> report on the role of nuclear models in the interpretation of data necessary for the analysis of fission and fusion reactors.

Due to our scant knowledge of the nature of nuclear forces, the physicist has been forced to assume an effective force of simple and well behaved form. This permits the introduction of a number of parameters. An example might be given for the well depth of the potential used in the Optical Model. The results of calculations using this well depth can vary widely depending on the form of the potential used. Furthermore, in most O-M calculations, all or some of the parameters are varied to optimize agreement between theory and experiment. As pointed out, these final parameters are not absolute since they required adjustment to correct for the inadequacies of the nuclear model.

Depending upon the phenomenological model chosen, and the approximation necessary for numerical simplicity, the results of evaluation can differ widely. This is especially true in areas where experimental data is lacking.

The central question which must be answered is: how important are the phenomenological aspects in defining the empirical data? A clear-cut answer to this question is difficult; however, one might try to interpret theoretical results which are independent of the parameters.

An often suggested possibility is to use a "realistic" force that reproduces the binding energy. This latter approach, while esthetically appealing, is affected by the inherent limitations of ordinary shell-model calculations.

Determining the force parameters or level density parameters from a least squares fit, while not as appealing as the purist would like, still remains attractive. This is especially true when such an analysis produces systematic trends in the parameters which may be reflected in our ideas concerning nuclear structure.

One must still be careful here also, since the many questions concerning the conditions which the parameters must satisfy have not been answered. Questions such as to the limit of uncertainty, the range of applicability and hidden correlation effects are only a few. Despite this unpropitious condition, the state of affairs is not beyond remedy.

First, we know that the models with all their drawbacks still have produced satisfactory results in the evaluation efforts. This is true even though a comparison of different calculational methods is made difficult by the impossibility of accurately determining the equivalence of corresponding analytical expressions.

In an attempt to alleviate many of the differences that result from the use of various formalisms and their respective codes, an effort has been undertaken in the USA to investigate the possibility of a "Master Code".

While a philia for the all purpose code (SUPRE-CØDE) has been with the theorists for some time, we are all aware that this would tax the capabilities of most computer complexes (not to speak of the evaluator). A possibility does exist, however, in the concept of a modular system; i.e., one in which data generated by Code A needed to carry out calculations in Code B could be stored on magnetic tapes, discs, etc. and called upon when necessary. An example is already seen in the transmission coefficients generated using a coupled-channel code which are used later in a Hauser-Feshbach calculation or other deductive analyses. Other necessary ingredients for model calculations such as compilations of binding energies, level schemes resonance parameters, level densities, etc. also lend themselves susceptible to the modular technique.

Now if one assumes that such a modular technique is feasible, the first step should then be to "modularize" the code, or combination of codes, which have proven to be most successful in the analysis of nuclear data. To ascertain which code(s) reflect this capability, the Nuclear Model Codes Subcommittee of CSEWG (USA) has undertaken the task of investigating certain questions that must be answered before any steps can be taken towards a MASTER CODE. This subcommittee consists of scientists from the major laboratories in the USA (ANL, BNL, HEDL, LASL, LLL, and ORNL) and private industrial firms such as General Electric, Westinghouse, etc.

Some of these questions which the subcommittee has embarked upon are:

- What should be the size limit on the code(s), assuming the computer type(s) has been established?
- 2. Kinds of incident particles  $(\gamma, n, p, \alpha, \text{ etc.})$  to be considered. Should the direct reactions of d,t, <sup>3</sup>He, heavy ions be considered? Should we include DWBA?
- 3. Energy range of incident particles is 20 30 MeV sufficient?
- 4. Should only one optical model subroutine be used for both spherical and deformed nuclei?
- 5. How can the numerical methods be improved? e.g. JUPITØR
- 6. Structure of code moduler (ease of model replacement i.e. subroutines interchangeability) e.g. ECIS 70/71. Type of information flow, libraries, data blocks. Retention of intermediate results for rerunning with minor parameter changes. Standardization of input and output between different modules.
- 7. Graphics display spline fitting least squares subroutines, etc.
- 8. Should Yrast levels be included?
- 9. Description of fission single hump, double hump, point-wise, etc. What about fission isomers?
- 10. Should the pre-compound process be explicitly included?
- 11. Absolute value and energy dependence of radiation widths. How should the v-ray strength functions be calculated?
- 12. Should angular distribution of all reaction products be included?
- 13. Should evaluation of parameter sets be undertaken?
- 14. Level density forms -

Of course the list of questions is not complete and it is obvious that a detailed treatment of any one item requires the expertise of specialists to that particular area.

A first phase study which included a comparison of some of the more recent statistical model codes such as GNASH (LASL), Uhl's HAUPT (BNL, LLL), HAUSER (HEDL) and TNG (ORNL) has already proven to be most helpful.

The success of the I-127 model comparison which involved an international effort on a voluntary basis, suggest that perhaps an International Model Codes Committee could be established wherein representatives from the members of IAEA could cooperate in such an undertaking.

In conclusion, although many difficult engineering problems remain to be faced, fission and fusion reactor engineering design is highly dependent upon the predictions of nuclear data evaluation. As such, these data must be drastically improved and the role of nuclear models cannot be over emphasized.

### Acknowledgement

The cooperation of E.D. Arthur (LASL), M. Divadeenam (BNL), C.Y. Fu (ORNL), D.G. Gardner (LLL), F.M. Mann (HEDL), R.E. Schenter (HEDL), P.G. Young (LASL), and members of NNCSC (BNL) is gratefully acknowledged.

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APPENDIX

Detailed Information on Nuclear Model Codes

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NAME OF PROGRAM: ABACUS-2 (revised)

AUTHOR: E. H. Auerbach

INSTITUTION: Brookhaven National Laboratory

DOCUMENTATION: BNL-6592 (unpublished) 1964

- <u>NATURE OF PHYSICAL PROBLEM</u>: ABACUS-2 is a combination of the Optical Model and the Hauser-Feshbach formalism. It has a 4 class capability.
  - <u>Class 1</u> Scattering by an optical potential: gives  $\sigma_{\rm T}^{},~\sigma_{\rm SE}^{},$  and  $\sigma_{\rm R}^{}$  only.
  - <u>Class 2</u> Computes the bound state radial wave function for a specific  $\ell$  and j.
  - <u>Class 3</u> Uses method of Class 1 to generate transmission coefficients for use in Hauser-Feshbach Theory. Computes  $\sigma_{\rm T}$ ,  $\sigma_{\rm SE}$ ,  $\sigma_{\rm CE}$ , and  $\sigma_{\rm nn}$ .
  - <u>Class 4</u> Calculates radial integrals from partial waves generated by Class 1 and 2.

A multidimensional search procedure is included for obtaining best optical model parameters.

PROGRAM LANGUAGE: Fortran IV

SIZE: 32 K

STATUS: Converted for PDP-10, CDC 6600, IBM-360

<u>Name of Code</u>: RAROMP (Regular and Reformulated Optical Model Program) <u>Author</u>: G. J. Pyle

Establishment: University of Minnesota, Minneapolis, Minnesota

Present Address - Phys. Dept., Univ. of Birmingham, England. <u>Nature of Problem Solved</u>: RAROMP is a general purpose search code, which performs optical model calculations using the reformulated optical

model and Greenlees et.al.

Program Language: FORTRAN II (CDC-6600)

<u>Size</u>: 32 K

- <u>Status</u>: Converted for PDP-10 at NNCSC BNL. Compiled and checking procedure in progress.
- <u>Name of Code</u>: ELIESE III (Program for Calculating of the Nuclear Cross Sections by Using Local and Non-Local Optical Models and Statistical Model).

Author: Sin-iti Igarasi

Establishment: Japan Atomic Energy Research Institute, Ibaraki-ken, Japan. <u>Nature of Problem Solved</u>: Calculates elastic, inelastic,  $n,\alpha$ ,  $p,\alpha$ , and n,pcross sections using the optical model and Hauser-Feshbach-Moldauer treatment.

Program Language: FORTRAN IV (IBM-360/75 and FACOM-230-60)

<u>Size</u>: 80 K

Status: Conversion to PDP-10 in progress.

Name of Code: ABACUS-NEARREX (Revised)

Author: P.A. Moldauer, and S. Zawadski

Establishment: Argonne National Laboratory

<u>Nature of Problem Solved</u>: Calculates elastic and inelastic, n,p, nY, n,f cross sections using Optical Model (ABACUS) and Hauser-Feshbach-Moldauer (NEARREX) theories.

Program Language: FORTRAN IV (IBM-360)

Size: 55 K (estimated)

Status: Received at NNCSC - BNL

<u>Name of Code</u>: MARE (A Fortran IV Code for Compound Nucleus Reaction Calculations in the Continuum).

Author(s): G. Reffo and M. Vaccari

Establishment: Comitato Nazionale Energia Nucleare, Bologna, Italy ..

Nature of Problem Solved: The evaporation theory and Blatt-Ewing formula

is used to calculate cross sections of the type (x:a), (x;a,b),

(x;a,b,n) where x, a, b can be neutrons, protons,  $\alpha$  particles, or

gamma rays; n stands for neutron.

Program Language: FORTRAN IV (IBM-360/75 and 7094)

Status: Converted for PDP-10 at NNCSC - BNL

A. Name of Program - WAVES

Author - Randall S. Caswell

Laboratory or institution - National Bureau of Standards

<u>Documentation</u> - NBS technical note 159 plus an improved manual (report number unknown).

# B. Purpose

<u>Nature of physical problem</u> - Waves solved for single-particle states in a potential well

Method of solution- Runge-Kutta integration method

<u>Restrictions, advantages and limitations</u> - Can solve for both bound and unbound single-particle states.

- 4. Other pertinent features
- C. Scope

Computer for which program is designed and others upon which it may be operable. We use it on the CDC 6600.

Program language - FØRTRAN

Size - 7000 words

Typical running time - one second

Does program contain overlays/chains/links -

Number and type of peripheral device required -None

Related auxiliary codes - None

A. <u>Name of Program</u> - JULIE

<u>Author</u> - R. H. Bassel, R.M. Drisco and C. R. Satchler <u>Laboratory or institution</u> - ORNL <u>Documentation</u> - ORNL-3240, Nucl. Phys. <u>55</u>. (1964)

B. Purpose

<u>Nature of physical problem</u> - Theory - Reaction Cross-Sections and angular distribution via direct interaction. <u>Method of solution</u> - Distorted-Wave- Born-Approximation <u>Restrictions, advantages and limitations</u> - Includes a variety of form factors as options. Variable radial mesh

C. Scope

Computer for which program is designed and others upon which it may be operable - IBM-360 Program language - FORTRAN-IV H Size - 500K bytes Typical running time -Does program contain overlays/chains/links - no overlays Number and type of peripheral device required - 4 scratch disks A. Name of Program - GENOA

Author - F.G. Perey

Laboratory or institution - ORNL

Documentation - none

# B. Purpose

<u>Nature of physical problem</u> - Theory - Optical Model Global Search <u>Method of solution</u> - Minimum chi-square

C. <u>Scope</u>

Computer for which program is designed and others upon which it

<u>may be operable</u> - IBM-360

Program language - FORTRAN IV H

Size - 270K bytes

Typical running time -

Does program contain overlays/chains/links - no overlays

Number and type of peripheral device required - no peripheral devices

NAME OF PROGRAM: STEPIT

Author: James H. Burrill, Jr.

Laboratory or Institution: Ohio University

Documentation: TNP-1966-2, May 10, 1966

### PURPOSE:

<u>Nature of Physical Problem - Theory</u>: STEPIT is a multi-dimensional search code.

Method of Solution: (See below)

Restrictions, Advantages and Limitations: Can search on any number of variables. STEPIT minimizes the function defined by the user's function subroutine using the cyclic relaxation method (see manual).

Other Pertinent Features: It is equally applicable to both linear and non-linear problems.

# SCOPE:

<u>Computer for which program is designed</u> and others upon which it may be operable: CDC 3600, CDC 6600, IBM 360

Program Language: Fortran

Size: 2300 words

Typical Running Time: Highly problem dependent

Does Program contain Overlays/Chains/Links: No

Number and Type of Peripheral Device Required: None

<u>Related Auxiliary codes</u>: This may be run with an arbitrary function subroutine.

<u>NAME OF PROGRAM</u>: (No name given) Subroutine available from author <u>Author</u>: B. E. Chi <u>Institution</u>: State University of New York at Albany <u>Documentation</u>: B. E. Chi, "Single-Particle Energy Levels in a Nilsson Well" (1967) S. G. Nilsson, Mat. Fys. Medd. Dan. Vid. Selsk <u>29</u>, (1955) No. 16.
<u>PURPOSE</u>: Calculation of single particle energy levels and wave function

<u>PURPOSE</u>: Calculation of single particle energy levels and wave function in a Nilsson model

Restriction: Neglecting the coupling of quantum number N due to  $\beta \rho^2 Y_{20}$ .

# SCOPE:

The code is adapted to PDP-10.

Program Language: Fortran IV

Size: (< 30 K decimal)

Typical Running Time: (< 5 sec.)</pre>

No Overlay, Chains and Links

No special peripheral device is required.

Related Auxiliary codes: None

#### NAME OF PROGRAM: SURF

Author: F. Fabbri, M. Marangoni, A. M. Saruis

Institute: Comitato Nazionale Energia Nucleare

# Documentation: RT/FI(69)29

B. Buck and A. D. Hill: Nuclear Physics <u>A95</u> (1967) 271
C. Mahaux and H. A. Weidenmüller, "Shell Model Approach to Nuclear Reactions"

# PURPOSE: Calculation of Photoreaction Cross Section in the One Particle-One Hole Continuum Approximation.

- 1. Theory Shell model approach to the photoreaction by using the one particle and one hole continuum approximation.
- 2. The coupled channeled equations of one particle and one hole continuum approximation is resolved by taking into account the isotopic spin mixing between T = 1 and T = 0, and the cross sections of photoreaction, inelastic and (p,n) reaction are calculated.
- 3. Restriction. The only photoreaction cross section from ground state is calculated. Number of channels is limited to 20.

### SCOPE:

The original code uses the <u>IBM-7094</u>, but the code is adapted to the CDC-6600.

Program Language: Fortran IV

<u>Size</u>: 104 K (oct)

Typical Running Time: 41 sec on CDC-6600

No Overlays, Chains and Links

Two tapes are required as scratch tape

No Related Auxiliary codes necessary
NAME OF PROGRAM: THRESH-2

AUTHOR: S. Pearlstein

ESTABLISHMENT: NNCSC/BNL

NATURE OF PHYSICAL PROBLEM: THRESH-2 calculates neutron induced cross sections in the energy range 0 - 20 MeV. A total of 19 reactions may be considered. These are n,n; n,2n; n,3n; n,p; n,d; n,t; n,He<sup>3</sup>; n,He<sup>4</sup>; n,np; n,nd; n,nt; n,nHe<sup>3</sup>; n,nHe<sup>4</sup>; n,pn; n,2p; n, $\alpha$ P; n,dn; n,p $\alpha$ . Either pointwise or fission spectrum average values may be calculated. It is best suited for nuclei in the range Z = 21 to 82.

PROGRAM LANGUAGE: Fortran IV

SIZE: 12 K

TYPICAL RUNNING TIME: 30 seconds per nuclide

STATUS: Available at ANL Code Center

REFERENCE: J. Nucl. Eng. 27, (1973) 81.

<u>Name of Code</u>: HAUPT (Program for Calculating Activation Cross Sections). <u>Author</u>: M. Uhl

Establishment: Institute for Radium Research and Nuclear Physics, Vienna, Austria.

<u>Nature of Problem Solved</u>: Program HAUPT calculates the activation cross section at prescribed levels of the final nucleus, the energy  $E_k$ , angular momentum  $I_k$ , and parity  $\pi_k$  for nuclear reactions of the type

$$T(a_0, a_1, a_2, \dots, a_n)E$$

where

T .... Target nucleus a<sub>0</sub>.... Projectile a<sub>1</sub>.... a<sub>n</sub> Emitted particle E .... Final nucleus.

The statistical model is employed with allowance for angular momentum and parity affects. Gamma decay is described by means of a cascade model.

Program Language: FORTRAN IV

Size: 26 K

Status: Converted for PDP-10 at NNCSC

GNASH - A Multipurpose Statistical Theory Code

- <u>CODE NAME</u>: GNASH (<u>Gamma-ray</u>, <u>N</u>eutron, and <u>A</u>sserted Particle <u>S</u>pectra from Neutron-Induced Reactions on <u>H</u>eavy Nuclei).
- AUTHORS: P. G. Young and E. D. Arthur
- COMPUTER: CDC 7600
- <u>CAPABILITY</u>: GNASH calculates level activation cross section, discrete gamma-ray cross sections, isomer ratios, and neutron, gamma-ray and charged-particle spectra from almost any combination of neutron-induced reactions up to 20 MeV or higher. The code handles de-excitation of up to ten nuclei in the decay sequence, and each decaying nucleus can emit up to six types of radiation (neutrons, gamma-rays, protons, alphas, etc.). A maximum of 50 discrete levels can be included for each residual nucleus formed in the calculation, which provides great flexibility in calculations of activation cross sections, isomer ratios, etc. Examples of reactions that can be handled in a single calculation are  $(n, \gamma)$ ,  $(n, n'\gamma)$ ,  $(n, \gamma n')$ ,  $(n, p\gamma)$ ,  $(n, np\gamma)$ ,  $(n, \Omega n\gamma)$ ,  $(n, 2n\gamma)$ ,  $(n, 3n\gamma)$ ,  $(n, 4n\gamma)$ , etc.
- METHOD: The calculation follows closely the statistical theory described by Uh1<sup>1</sup>. Widths for particle decay are computed from externally calculated optical model transmission coefficients. Gamma-ray widths are calculated using either the Weisskopf single-particle approximation<sup>2</sup> or the Brink-Axel giant dipole resonance model.<sup>3</sup> Gamma-ray emission by electric and magnetic dipole or quadrupole transitions are allowed, and gamma-ray cascades are followed in detail. The Gilbert and Cameron<sup>4</sup> form of level density function is used and is matched with inputted discrete data for up to 50 lowlying states per residual nucleus. A simple pre-equilibrium model is used to correct particle spectra and level excita-

tion cross sections for semi-direct processes.

# References

- 1. M. Uhl, Acta Physica Aust. <u>31</u>, (1970) 245.
- J. M. Blatt and V. F. Weisskopf, "Theoretical Nuclear Physics", Wiley, New York, (1952).
- D. M. Brink, Thesis, Oxford University, 1955; P. Axel, Phys. Rev. <u>126</u>, (1962) 671.
- 4. A Gilbert and A. G. W. Cameron, Can. J. Phys. <u>43</u>, (1965) 1446.

Name of Code: HAUSER

Author: F. M. Mann

Establishment: Hanford Engineering Development Laboratory, Richland, WA.

Nature of Problem Solved: Program HAUSER calculates the total reaction cross section for T(a,bc)F where T is the target nucleus, a is the projectile (any particle-charged or uncharged), b and c are emitted particles or gamma rays, and F is the final nucleus. The statistical model is employed with allowance for angular momentum and parity effects. The transmission coefficients can either be calculated (without spin-orbit interaction) or read-in. Width fluctuation corrections can be included through the method of Tepel, Hofmann and Weidenmueller. Cross sections can be printed for discrete states, two-body or three-body reactions.

## Program Language: FORTRAN IV

- <u>Size</u>: 170 K for 7 values of bc, 6 values of b, 100 discrete states. Can be considerably reduced by reducing size of tables.
- <u>Status</u>: Has run on IBM 370 and CDC 6600 and 7600. Program being modified to include fission.

<u>NAME OF PROGRAM</u>: CINDY - Computation of total and differential cross section for compound nuclear reactions of the type (a,a), (a,a'), (a,b), (a,Y), (a,Y-Y), (a,bY) and (a,bY-Y).

<u>AUTHOR(S)</u>: E. Sheldon (Lowell Tech. Inst. Lowell, Mass.) V. C. Rogers (Brigham Young Univ., Provo, Utah)

DOCUMENTATION: Comp. Phys. Comm. 6, (1973) 99 (North Holland Publ.)

NATURE OF PHYSICAL PROBLEM: Evaluation of total and differential cross sections in absolute and normalized form for (a,a), (a,a'), (a,b), (a,γ), (a,γ-γ), (a,bγ) and (a,bγ-γ) reactions using statistical compound-nucleus theory, with spinorbit interaction and/or the Moldauer levelwidth fluctuation correction. The program has been extended to calculate radiative capture (in competing transitions), to take account of competing channels to a continuum of residual states, and to automatically calculate any required transmission coefficients from prespecified optical-potential parameters.

PROGRAM LANGUAGE: Fortran IV

COMPUTER: IBM/370 and IBM/360

SIZE: 30 K

NO MAGNETIC TAPES REQUIRED

NO OVERLAY

TYPICAL RUNNING TIME: Varies - 1 min. for uncomplicated problem to more than 1 hr. for sequential calculations of many exit channels and high momentum.

STATUS: Converted for use on CDC 6600 BNL

<u>Name of Code</u>: TNG (A Two-Step Hauser-Feshbach Code with Precompound Decays and Gamma-Ray Cascades)

Computer for which Code is Designed: IBM 360/75 and 360/91

Nature of Physical Problems Solved: The code is designed for calculating nuclear reaction cross sections below 20 MeV. Binaryreaction, tertiary-reaction and gamma-ray-production cross sections such as  $(n, \gamma)$ , (n, p), (n, 2n),  $(n, n' \gamma)$ ,  $(n, On \gamma)$  may be calculated. Energy distributions of secondary particles and gamma rays may be output in ENDF/B formats. Angular distributions of the first outgoing particles may be output in terms of Legendre coefficients.

Method of Solution: The Hauser-Feshbach formula<sup>2</sup> for compound binary reactions is extended to include tertiary reactions. Sequential decays without correlation between the two outgoing particles are assumed. Transmission coefficients needed for each step of the sequential decays are calculated with an in-house optical model without spin-orbit coupling. Binary-reaction part of the code, including width-fluctuation corrections, is based on the ORNL Hauser-Feshbach code HELENE.<sup>3</sup> A precompound model<sup>4</sup> may be included as a correction to the energy distributions of the first outgoing particles. Gamma-ray competition with the second outgoing particles and the gamma-ray-cascades calculations are spin- and parity-dependent, thus sensitive to the angular momentum effects of the Hauser-Feshbach method. Gamma-ray branching ratios, if not available experimentally, are estimated from the tails of electric giant dipole resonances.<sup>5</sup> The parity selection rule of electric dipole transitions may be partially relaxed as a means of including magnetic dipole transitions.

<u>Restriction on Complexity</u>: Present dimensioning restricts a maximum of three types of binary particles and three types of tertiary particles.

Representative running time: The running time is roughly proportional

to  $(E \ge \Delta E)^2$  where E is the incident neutron energy and  $\Delta E$  the continuum bin width. For E = 14 MeV,  $\Delta E = 0.2$  MeV and a case that includes (n,n'x), (n,px) and (n, $\alpha$ x) with x = Y, n, p, or  $\alpha$ , and gammaray-cascades for every residual nucleus, the running time would be roughly two minutes on IBM 360/91.

<u>Related or Auxiliary Programs</u>: Collective excitation cross sections from measurements and/or calculations may be input to TNG so that the collective effects are included in the calculated gamma-ray-production cross sections.

Status: In use at ORNL.

Machine Requirements: 300 K bytes of core.

<u>Materials available</u>: Complete code package will be available by July 1, 1975 from the Radiation Shielding Information Center at the Oak Ridge National Laboratory.

<u>Acknowledgements</u>: Work funded by the Defense Nuclear Agency and the Atomic Energy Agency under contract with the Union Carbide Corporation.

### References:

- C. Y. Fu, "TNG, A Two-Step Hauser-Feshbach Code with Precompound Decays and Gamma-Ray Cascades," Technical Memorandum, Oak Ridge National Laboratory (in preparation).
- W. Hauser and H. Feshbach, Phys. Rev. <u>87</u>, (1952) 366. A. M. Lane and R. G. Thomas, Rev. Mod. Phys. <u>30</u>, (1958) 257.
- S. K. Penny, "HELENE A Computer Program to Calculate Nuclear Cross Sections Employing the Hauser-Feshbach Model, Porter-Thomas Width Fluctuation, and Continuum States," ORNL-TM-2590, Oak Ridge National Laboratory (1969).
- 4. J. J. Griffin, Phys. Rev. Lett. <u>17</u>, (1966) 478.
  M. Blann, Phys. Rev. Lett. <u>21</u>, (1968) 1357.
  M. Blann, Nucl. Phys. <u>A213</u>, (1973) 570.
- P. Axel, Phys. Rev. <u>126</u>, (1962) 671.
   P. Oliva and D. Prosperi, Nuova Cimento ILB, (1967) 161.

AUTHOR: F. Schmittroth

LABORATORY OR INSTITUTION: HEDL

DOCUMENTATION: HEDL-TME 71-106 describes theory, no code documentation

#### B. PURPOSE

NATURE OF PHYSICAL PROGRAM: Radiative Neutron Capture Cross Section METHOD OF SOLUTION: Statistical Theory with

- a. optical model
- b. width fluctuations
- c. special attention to continuum regions
- d. corrections for  $(n, 2\gamma)$  and direct reactions

RESTRICTIONS, ADVANTAGES AND LIMITATIONS: up to 20 inelastic levels

C. SCOPE

COMPUTER FOR WHICH PROGRAM IS DESIGNED AND OTHERS UPON WHICH IT MAY BE OPERABLE: UNIVAC 1108. Will be converted to CYBER 74 (CDC 6600).

PROGRAM LANGUAGE: Fortran IV

SIZE: 50 K words

TYPICAL RUNNING TIME: 1 minute for 10 energies and 1 isotope

DOES PROGRAM CONTAIN OVERLAYS/CHAINS/LINKS: no overlays

NUMBER AND TYPE OF PERIPHERAL DEVICE REQUIRED: no peripheral de-

vices except for input.

AUTHOR: T. von Egidy

ESTABLISHMENT: Physics Department Technische Hochschule Munich, Federal Republic of Germany

<u>NATURE OF PROBLEM SOLVED</u>: The capture gamma-ray spectrum, the multiplicity, the population of levels (isomer ratio) and the line density is calculated using formulae for the level density and transition probability.

PROGRAM LANGUAGE: Fortran IV

SIZE: Approximately 10 K

STATUS: Converted to PDP-10

<u>NAME OF CODE</u>: SURF\* - Program for the coupled-channel calculation of the photoreaction cross sections in the one particle-one hole continuum approximation RT/FI(69)20

AUTHORS: F. Fabbri, M. Marangani, and A. M. Saruis

ESTABLISHMENT: CNEN - Bologna, Italy

<u>NATURE OF PROBLEM SOLVED</u>: The program calculates the dipole photoreaction cross sections of doubly closed shell nuclei in the 1p-1h continuum approximation.

PROGRAM LANGUAGE: Fortran IV IBM 7094

SIZE: Overlay version

STATUS: Received at NNCSC and being converted to PDP-10

\*Please note that the authors of SURF suggest that all requests for this code be sent to them directly. <u>NAME OF CODE</u>: DIRCO\* - Fortran program for calculation of dipole raditive capture cross sections according to direct and collective models RT/FT(71)29

AUTHORS: F. Fabbri, G. Longo and F. Saporetti

<u>NATURE OF PROBLEM SOLVED</u>: The program calculates the direct and collective capture cross sections for individual single-particle bound states at a given incident nucleon energy. The total cross section is given as the sum of the contributions over all possible final states. The theoretical formalisms are described in References 1 to 4.

PROGRAM LANGUAGE: Fortran IV IBM 360/75

STATUS: Being converted and checked out for PDP-10

- <u>REFERENCES</u>: 1. A. M. Lane: Nucl. Phys. <u>11</u>, (1959) 625. A. M. Lane and J. E. Lynn: Nucl. Phys. <u>11</u>, (1959) 646.
  - 2. C. F. Clement, A. M. Lane and J. R. Rook: Nucl. Phys. <u>66</u>, (1965) 273.
  - 3. G. Longo and F. Saporetti: Nuovo Cimento 52B, (1967) 539.
  - 4. G. Longo and F. Saporetti: Nuovo Cimento 56B, (1968) 264.

\*Please note that the authors of DIRCO suggest that all requests for this code be sent to them directly. Name of Code: JANE

Author: J.M. Ferguson

Establishment - Naval Defense Radiological Lab., NRDLCP-68-9

Present Address: LLL., Calif.

## Nature of Problem Solved

Prog. JANE calculates cross sections for (n,n'), (n,p), and  $(n,\alpha)$  reactions along with angular distributions for secondary neutrons and Y-rays from the (n,n') reaction.

The calculations are performed with a combustion of optical model and Hauser-Feshbach routines, with Moldauer type width fluctuation corrections.

Program Language: FORTRAN IV

<u>Size</u>: 32 k

Status: Converted for PDP-10 /CDC 6600 at BNL.

A. Name of Program- HELENE

Author - S. K. Penny

Laboratory or institution - ORNL

Documentation - ORNL-TM-2590

## B. Purpose

<u>Nature of physical problem</u> - Theory - Reaction Cross Sections and angular distribution via compound nucleus <u>Method of solution</u> - Hauser-Feshbach with Width Fluctuation corrections, optical model <u>Restrictions, advantages and limitations</u> - Includes charged particle competition, continuum states, and capture.

## C. <u>Scope</u>

<u>Computer for which program is designed and others upon which it</u> <u>may be operable</u> - IBM-360 <u>Program language</u> - FORTRAN-IV H <u>Size</u> - 256K bytes <u>Typical running time</u> -<u>Does program contain overlays/chains/links</u> - no overlays <u>Number and type of peripheral device required</u> - no peripheral devices A. Name of Program - HELGA

<u>Author</u> - S. K. Penny <u>Laboratory or institution</u> - ORNL Documentation - none

B. Purpose

<u>Nature of physical problem</u> - Theory - Reaction Cross-Sections and angular distribution via compound nucleus and gamma-ray cascade. <u>Method of solution</u> - Hauser-Feshbach with Width Fluctuation corrections, optical model, statistical model.

<u>Restrictions, advantages and limitations</u> - Angular distributions of gamma-rays are not computed, includes charged particles and capture competition and continuum states

Other pertinent features - Has three regions of excitation spectrum, discrete, quasi-discrete and continuum. Quasi-discrete region contributions are weighted to give effectively the same number of levels predicted by the continuum model in that energy region. Direct interaction cross-sections may be read as input to add to compound numbers cross-sections. The discrete and quasi-discrete cascade gamma-rays are computed but the continuum gamma-ray cascades are read as input computed with program DUCAL. C. Scope

Computer for which program is designed and others upon which it may

be operable - IBM-360

Program language - FORTRAN-IV H

Size - 740K bytes

Typical running time -

Does program contain overlays/chains/links - no overlays

Number and type of peripheral device required - no peripheral devices

Related auxiliary codes - DUCAL

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A. Name of Program - SPECTIO

Author - P.G. Young and M. Drake

Institution - Los Alamos Scientific Laboratory

<u>Documentation</u> - P. Young and M. Drake, official memo of Los Alamos Scientific Laboratory, August 13, 1968.

E. S. Troubetzkoy, Physical Review, 122, (1961) 212.

B. Purpose - Calculation of inelastic gamma-ray spectra.

Theory - Statistical theory.

Method of solution - refer to the above documentation.

<u>Restriction</u> - Take into account the discrete level when neutron channel is open, the Y channel is closed. Three types of density formula  $\rho \sim E^{-2} \exp(2\sqrt{a})$  $\rho \sim \exp(E/a)$  and  $\rho \sim \exp(2\sqrt{aE})$  are used.

C. Scope

The code is adapted to PDP-10 machine except for plotting subroutine. <u>Program language</u>: FORTRAN IV <u>Size</u>: (< 30 k decimal) <u>Typical running time</u>: < 10 sec in PDP-10. No overlays, chains and links. No special peripheral devices are required. <u>Related auxiliary</u> codes - none. Name of Program - FISPRO II

<u>Author</u>: V. Benzi, G. C. Panini, and G. Reffo <u>Establishment</u>: C.N.E.N. Bologna, Ref. CEC (69) 24

#### Purpose

A Hauser-Feshbach program which calculates radiative capture crosssection. Includes corrections for n-2gamma, direct, and collective capture but does not include width-fluctuation corrections.

Transmission coefficients may be read from cards, or program will calculate them from either a black-nucleus model or from an internal optical-model program which uses various forms for a spherically symmetric potential.

Includes the effect of inelastic-scattering to both known and unknown levels in the target nucleus.

#### SCOPE

<u>Program Language</u>: A FORTRAN-IV program which requires about 13 K words for storage on a 1108 UNIVAC. No overlays, or mass storage devices are required.

The program is self contained.

<u>Running Time</u>: 0.3-0.5 sec. per energy point when transmission coefficients are read or are calculated by the black-nucleus model. The opticalmodel calculations and the n-2Y corrections can each increase this time by 10.0 sec. Author(s): C. K. Cline and M. Blann

Establishment: Nuclear Structure Lab., University of Rochester, Rochester, New York

## NATURE OF PROBLEM SOLVED:

The program carries out calculations with a pre-equilibrium statistical model as outlined in References 1 and 2. Numerical techniques are used to solve a set of coupled differential equations which yields the mitantaneous particle spectra. Integrating these spectra produces the total spectrum of particles emitted up to any time.

Cutting off the integration when equilibrium is reached leads to the total pre-equilibrium spectrum.

The program is capable of calculating the spectra for emitted particles of arbitrary spin and nucleon number.

### PROGRAM LANGUAGE: Fortran IV (PDP-10)

Size: Less than 20 K

Status: Adapted to PDP-10 NNCSC

### **REFERENCES:**

- 1. J. J. Griffin, Phys. Rev. Lett. 17, (1966) 478.
- 2. C. K. Cline and M. Blann, Nucl. Phys. A172, (1971) 225.
- 3. C. K. Cline, Nucl. Phys. A193, (1972) 417.
- 4. F. C. Williams, Jr., Nucl. Phys. A166, (1971) 231.
- 5. C. K. Cline, Nucl. Phys. A195, (1972) 353.
- 6. C. Kalbach-Cline, Nucl. Phys. <u>A210</u>, (1973) 590.
- 7. I. Ribansky, P. Oblozinsky and E. Bětak, Nucl. Physics <u>A205</u>, (1973) 545.

NAME OF CODE: PRECØ-A

Author: C. Kalbach

Establishment: C. E. N. Saclay, France

Present Address: University of Tennessee, Knoxville, Tenn.

NATURE OF PROBLEM SOLVED:

<u>Pre-equilibrium model</u>: This code is an extension of PRECØN/PRECØM. The formalism is essentially that contained in Reference 1 with the inclusion of refinements described in References 2 - 6.

PROGRAM LANGUAGE: Fortran IV

Machine: IBM 360/65 or CDC 6600/7600

Size: Approx. 20 K

Status: Adapted to PDP-10

**REFERENCES:** 

- 1. J. J. Griffin, Phys. Rev. Lett. 17, (1966) 478.
- 2. C. K. Cline and M. Blann, Nucl. Phys. A172, (1971) 225.
- 3. C. K. Cline, Nucl. Phys. A193, (1972) 417.
- 4. F. C. Williams, Jr., Nucl. Phys. A166, (1971) 231.
- 5. C. K. Cline, Nucl. Phys. <u>A195</u>, (1972) 353.
- 6. C. Kalbach-Cline, Nucl. Phys. <u>A210</u>, (1973) 590.
- Ribansky, P. Oblozinsky and E. Bétak, Nucl. Phys. <u>A205</u>, (1973) 545.

Review Paper No. 1b

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

M.K. Mehta Bhabha Atomic Research Centre, Bombay- 400085, India.

## ABSTRACT

The situation in developing countries is reviewed first by examining the motivation for such work and then by setting up a few criteria necessary for carrying out data evaluation pregrammes. The case for one country-India is discussed in detail under these criteria and general inferences are drawn from this. Recommendations are made based on this review to bring about interactions between the basic nuclear theorists and nuclear data evaluation groups in developing countries.

### A. INTRODUCTION

If one does not carefully read the title of the introductory paper that I am supposed to prepare, one would wonder why there are two introductory review papers with a similar title. However the words "developing countries" would bail me out, especially at this Centre which has done so much in contributing to and encouraging high quality theoretical work in the developing countries in the fields of nuclear physics, high energy and particle physics and solid state physics.

Having listened to the previous speaker all of us would agree that nuclear theories and models have a very important role to play in practical evaluation of neutron nuclear data needed for fission and fusion reactor programmes. It is also very clear that the nuclear data evaluator has to be familiar with the scope and limitations of a theory or model that he is using, otherwise the credibility and confidence in the numbers that he generates become questionable. The previous speaker has vary ably and extensively covered the status of various theories, their role, importance and limitations. These are basic aspects of physics and are invariant with respect to the state of development of a country.

With this background, the purpose of the present paper is present you with a review of the situation as to what extent data evaluation work, incorporating data prediction by the use of the proper nuclear theory, can be carried out in a useful and relevant manner in a developing country. In this respect this paper will deal more with policies, scope, limitations and erganisation of such work in a developing country.\* In order to do this, a set of criteria is suggested which can be used to svaluate the motivation, petential, and problems for such programmes in these countries. These criteria are used to review the situation in India, - the auther being familiar only with that "developing country".

It is not necessary here, in the context of the energy situation in the world to dwell on the importance of atomic power programmes especially in the developing countries. We will assume that a power reactor programme is in existence. The reactors would be outright purchases from commercial firms, copies of already working prototypes put up with technical collaboration with the countries concerned, or of totally indigenous design. Even if they belong to one of the first two categories, cur experience has shown that local conditions and constraints enforce so called 'minor'medifications at the commissioning stage or later while servicing and mainteining the reactor at the optimum power production level. This would require

<sup>\*</sup> The words "developing countries" are rather ambiguous and are sometimes used to mean "small countries". In the present paper these words are used to mean countries whose economies are not fully developed and who have limited economic resources, trained manpower or both.

new calculations involving basic cross sections for different structure materials. In a few cases the necessary modifications may involve the fissile and fertile materials too. The last category, i.e. the indigenous design, of course, will require full fledge reactor physics calculations involving basic cross sections. The point being made here is that it is essential for any country which has any reactor programme, to maintain a trained group of people who can do data evaluation \* for input to their reactor physicists even when the reactors are commercially supplied with fixed period guarantees or are copies of well tested working models put up with technical collaboration. A well trained data evaluation group implies familiarity and understanding of the experimental techniques as well as the theories. Apart from modification of computer codes, necessary to incorporate latest development of the theory. it may be necessary to adopt the code to the available computer which may be different from the one for which the computer programme was originally written. The group may have to write an entirely new computer programme. Thus for a developing country, given a power reactor programme we can accept that the need for a sizable data evaluation and prediction effort is well established.

### B. <u>CRITERIA</u>

At this stage it would be useful to develop a few criteria which should be satisfied for a developing country to establish a meaningful and sizable effort in data evaluation and prediction. The foremest of such criteria would be the fact that the country should not become tee dependent on external inputs. Such inputs should be at the same or a slightly higher level than that of normal international interaction in academic fields. Agencies like the IAEA can certainly help in providing the right kind of support but no country should and would expect spoon feeding. Bilateral agreements are generally fermulated on give and take basis. Thus the policy in this matter should be directed at developing indigenously as much know-how as the manpower resources would permit, utilising the existent expertise. It is here that the International agencies can help by previding the necessary resources in the form of funds, equipment, and expertise. Let us look at what expertise is necessary to develop a data evaluation prediction programme strong enough to be consistent with the scope of the power reactor programme in a developing country.

(1) Existence of a strong school of basic theoretical work in Nuclear <u>Physics:</u> Having listened to the previous paper there is no need to emphasise this point. A group of people who themselves are contributing to the progress and pace of research in nuclear theory would be an asset in developing the applied aspects relevant to data evaluation and prediction. Some of these scientists themselves can take over the applied work or can help in training the data workers to become aware of the developments in the field and help in innovating different techniques and in writing the corresponding computer programmes.

<sup>\*</sup> From now on the words "data evaluation" will include data prediction also.

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(ii) Existence of data evaluation groups: As discussed under A above such a group is absolutely essential for any country which has a power reactor programme. An ideal group would be a proper mix of experimental and theoretical nuclear physicists as well as reactor physicists. If such an ideal group does exist the criterien(iii) below becomes redundant. However this is not the case in most of the developing countries.

# (iii) Interaction between the theorists -(i) above - and the data

workers - (11) above: A strong interaction between the two groups (i) and (ii) is essential for any sizeble indigenous and meaningful data effort. For a "developed" country with a good size reactor programme the group (11) itself has enough inputs to attract mambers of group (1) to totally go over to data work and become a part of group (ii). This will automatically meet criterion (iii). A big enough reactor programme with abundance of economic and manpower resources would automatically lead to this condition. However for a developing country with limited economic and trained manpewer resources this is not so. It becomes very important then to bring about the interaction between the pure theorists and the data workers. Such an interaction would give rise to (a) development of applied theory te solve specific data prediction problems; (b) training of data workers in basic nuclear theory and (c) development of comprehensive computer codes. This last of course has limitations imposed by the available computer.

### C. SITUATION IN A DEVELOPING COUNTRY

Having established the conditions for development of applied nuclear theory and computer codes for data evaluation in a developing country, let us examine a country under these criteria. Being familiar with the conditions in India, I have chesen that as a test case.

The present Indian power reactor programme in its first phase is based on CANDU type of reactors. Work on three power stations such employing two reactors of around 200 MWe each has progressed to different levels for each station. Apart from this a power station employing two light water-enriched uranium reactors purchased from GE has been in operation for a few years now. A fast breeder prototype reactor is under construction. Indian interests include thermal as well as fast power reactors including breeder reactors and thorium fuel cycles. Thus a strong motivation exist for nuclear data evaluation work. Taking the three criteria discussed in 8 above and applying them one by one to the Indian case we get the following picture:

(i) <u>Work in the field of basic nuclear theory</u>: A number of strong schools exist in India which have made valuable contributions in the field of microscopic nuclear structure theories. The Physical Research Laboratory at Ahmedabad, the Saha Institute of Nuclear Physics at Calcutte and the Tata Institute of Fundamental Research at Bombay have a long tradition of theoretical work and each has at present a small but very competent group of scientists who are active in the field. A large number of them have had associations with this Centre.

Self consistent deformed Hartree Fock calculations using projection techniques, extensive multishell calculations utilising realistic nuclear-nucleon interactions and calculation of two body matrix elements have been the major areas of work at these places. These basic research programmes have generated a number of computer codes ranging from simple least square fits and angular momentum coefficient codes to the sephistication of Hartree-Fock-Bogolubev calculation. Although the data evaluation work does not directly involve these types of calculations, these research programmes, apart from generating the knowhew for writing sophisticated computer codes, have also produced the trained manpower which is available. At the Bhabha Atomic Research Centre to which I belong, we have a strong group which has been carrying out basic research, theoretical as well as experimental, in the field of nuclear fission. As far as the relevance to topics to be covered at this meeting are concerned this group has made sizable contributions in the field of statistical and fission theory. Later at this meeting I shall report the contributed paper from this group.

Smaller but significant theoretical work is being carried out in the fields of reaction theories and models at the Saha Institute, BARC, TIFR, the Banaras Hindu University and the Aligarh Muslim University. The major areas covered are the development and application of DWBA fermalism to include deuteron break-up channel through coupled channel techniques, cluster knock-out and three body reactions at medium energies, pien-nucleus interactions and microscopic calculations for optical potentials. All of this work requires extensive computer codes which are written by the persons involved. It has also generated the expertise in theories and models relevant to data evaluation work, e.g., optical, direct reactions and statistical models and fission theory. This provides a pool of manpower which can be drawn upon either for lectures meant for data evaluators and/or to develop proper technique to solve specific data problems.

This is not the place to go into the details of the actual research programmes of these groups but it is clear from this that criterion (i) is well satisfied for India.

(ii) Existence of Data Evaluation Groups: In order to meet the data needs for the reactor physicists in India, the data evaluation work is incorporated in the pregramme of two Reactor Physics Sections, one at the BARC whose main interests are tackling the problems of the light water-enriched uranium station already in operation as well as all the work connected with the CANDU type of power stations. The other Reactor Physics Section is attached to the Reactor Research Centre located near Madras whose main interests are centered on fast reactors. However the areas of work of each of these groups are not exclusively defined and there is a considerable overlap and interaction between the two groups. The following is a brief summary of the type of work these groups are deing.

Both the data evaluation groups are doing data prediction as well as data processing work. The materials for which this is done include fissile and fertile materials(U, Pu, Th), structural materials like Fe, Cr, Ni, Mo etc., coolant materials like Na and He, centrol materials like B and Ta, fuel diluents like O, C, N and fission product nuclides. For the processing work data libraries like ENDF(8), KEDAK(1970) and the Cadarache files are used. It is planned to set up a data library at the Reactor Research Centre which will incorporate the result of these efforts.

For the data "prediction" work the total, electic and inelastic cross sections have been calculated through the spherical optical model utilising the computer code ABACUS which was medified to run on the CDC-3600 computer available to the group at BARC. It involved the writing of some new subrountines. Compound nucleus contributions and cross sections for level excitations are calculated through the Hauserfeshbach approach. Another code NEAR-REX is utilised for calculating level excitations, and capture and fission cross sections. The width fluctuation corrections are incorporated in this programme, the input for which are transmission coefficients generated by ABACUS.

The inelastic scattering cross sections are needed for the high energy range-especially for fast reactors, as the inelastic scattering is the main mechanism through which neutrons loose their energy in this range. For these energies, inelastic scattering can be described well by the evaperation model which needs the "nuclear temperature" parameters as input. A computer programme INSCAT is written to calculate the inelastic transfer cross sections for about 16 nuclides which utilises the evaporation model for energies greater than 2 MeV. Below 2 MeV the group has not been able to do these calculations. I quote-"due to the nonavailability of reliable nuclear parameters for the evaporation model and the reliable date on the resolved excited levels for various nuclides."

The differential neutron scattering cross section data available from experiments have to be processed suitably for utilisation in neutronics calculations.

The "processing" programmes of these groups include evaluation of capture,fission,scattering and total cross sections in the resolved and unresolved resonance regions with single and multi level Breit-Wigner theory, Lane and Lynn theory of unresolved resonances and Adler and Adler theory of resolved resonances. A computer programme,LEGC, is written to generate Legendre coefficients from measured angular distributions for elastically scattered neutrons. These coefficients at various energies are useful in generating transfer matrices for elastic scattering which is done by the computer programme TRALEG. These transfer matrices are needed for fast reactor core calculations end for shielding design.

A number of computer codes are written to perform specific data evaluation of computer codes are written to perform specific data evaluation of processing; for example evaluation of fission widths of 1<sup>+</sup> states in <sup>239</sup>Pu resonances and updating of intermediate resonance parameters by fitting the measured  $^{+}$ C <sup>+</sup> values to the calculated values is done by a code named INCREP. Another code, RANRES, generates paudo random resonances in unresolved resonance region which takes into account the intermediate structure observed in the fission

widths for <sup>239</sup>Pu. These psudo rendom resonances based on the statistics determined in the resolved region are used to calculate effective cross-sections in the unresolved region. Similar calculations are being done for <sup>233</sup>U also. A processing code EFFCROSS generates multigroup cross section sets for a given composition and temperature of materials. The code DGPSEL generates self shielding factors for neutron capture, fission and scattering processes in both the resolved and unresolved resonance regions. Thus it can be seen that a sizeble data evaluation effort is current in India and a large number of computer programmes are written for this.

(iii) Interaction between the basis theorists and the data workers: Having dealt with the criteria (1) &(11), in the case of India, we find that both of them are well satisfied. However the situation for the important criterion of strong interaction between the two groups (i) & (ii) is far from satisfactory. In discussing their work with the evaluation group, one can easily find areas where an interaction with basic theorists could either fill a gap or make the computer programmes more efficient or both. The background of a large majority of persons in these evaluation groups is more Reactor Physics than Nuclear Physics and hence the interaction with basis nuclear theorists would contribute towards the basic understanding of the theories used. On the otherhand the basic theory workers in India are not even aware of the need and the petential for the contribution that they can make in this applied work. Even when there was awareness there has been an apathy towards this type of work which is assumed to be not sufficiently interesting to motivate the basic theorist. However this situation has changed in the recent past and now there is willingness to do such applied work, as part of their normal research programmes. In fact new we have a basic nuclear structure physicist working with our Reactor Physics Section.

At this point it may be right to generalise the case to the majority of developing countries. In many such countries due to the lack of experimental facilities and limited availability of funds a bright young physicist is generally more attracted to work in the areas of theoretical research. Because of this many of the countries are likely to have one or more active groups in basic theoretical research in nuclear physics or high energy physics or both. Thus criterion(i) is likely to be met to a limited extent in many countries. However there is no information regarding the applied theoretical effort in the data evaluation fields in other developing countries. It is likely that such an effort does exist on a smaller scale than that in India.

### D. <u>RECOMMENDATIONS</u>

Based on the rather brief review of the situation in developing countries above, some general inferences can be drawn and a few specific recommendations can be made. It is evident that in developing countries good potential does exist for development of applied theory and corresponding computer codes. Scope of such work depends to a large extent on the reactor programme of each country. It is quite extensive for a country like India especially because of the possibilities of developing the thorium fuel cycle. It is essential

that this potential is fully developed in the country to enable it to meet the demand made by its own power reactor programmes. In order to bring this about, good interaction has to be established between the basic theory workers and the nuclear data workers in the developing countries. One way to do this would be to hold workshops where basic theorists as well as data workers can participate, the primery programme for which can include lectures and discussions on developments in nuclear theory relevant to data work. On the other hand it should also include a few seminars on specific problems that data workers face which would be educative to the basic theorists. Some of the lecturers in the basic theory, as well as the main body of the participants should be drawn from the developing countries. However participation from the "developed" countries with extensive programmes is also essential at such a workshop, which should not be just tutorials meant for training inexperienced workers. A properly organised and conducted workshop may also result in new ideas and techniques relevant to development of applied theories.

India would be willing to participate in such a workshop and would be able to provide lecturers for the selected topics.

Before concluding I would like to draw attention to an important constraint namely the availability of a large size computer. This involves financial resources of a country, as against the trained manpewer resources considered in the above discussion. Substantial financial aid would be needed to set up such computers. One solution could be large regional computing centres supported by international agencies like the IAEA.

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Statistical Theory of Neutron Nuclear Reactions $^{\star}$ 

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# ABSTRACT

The statistical theory of average neutron nucleus reaction cross sections is reviewed with emphasis on the justification of the Hauser Feshbach formula and its modifications for situations including isolated compound nucleus resonances, overlapping and interfering resonances, the competition of compound and direct reactions, and continuous treatment of residual nuclear states.

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# 1. STATISTICAL THEORY AND THE OPTICAL MODEL

The fundamental description of a quantum mechanical system, such as the atomic nucleus is provided by the wave function  $\psi$  which is obtained from the solution of the Schrödinger equation  $(H-E)\psi=0$ , where H is the Hamiltonian energy operator, which includes all kinetic and interaction energies of the system, and E is the energy of the system. Even in a relatively light nucleus, the many interaction terms between the nuclear constituents give rise to strong and rapid variations of  $\psi$ when the energy is varied at excitations of several MeV or higher, where neutron induced reactions can take place. The details of these variations are often difficult to ascertain theoretically and they are often irrelevant to nuclear power applications because they are washed out by Doppler broadening and by effective flux averaging. It is therefore useful to treat these variations statistically, that is to say, by discussing energy averages of relevant quantities, such as cross sections.

For the discussion of scattering and reactions we are interested only in the asymptotic wave function which is specified by the S-matrix whose typical component  $S_{cd}$  is the coefficient of the outgoing wave in channel d when a unit flux plane wave is incident only in channel c. The S-matrix is required to be symmetric and unitary because of timereversal invarience and flux conservation, and its elements completely determine all observable cross-sections. For example the differential cross section for scattering from a neutron channel c to the same or any other channel d has the form

$$\frac{d\sigma_{cd}(\Theta)}{d\Omega} = \sum_{L} P_{L}(\cos\Theta) \sum_{c,d'} f_{Lcc'dd'} Re \left[ (\delta_{cc'} - S_{cc'}) (\delta_{dd'} - S_{dd'}^{*}) \right]$$

$$f_{Lcc'dd'} = (-1)^{S} c^{-S} d \frac{\chi_{c}^{2}}{4(2s_{c}+1)} \sum_{\ell_{c'},\ell_{d'},J_{1}J_{2}} i^{\ell_{c}-\ell_{c'}+\ell_{d'}-\ell_{d'}-\ell_{d'}-2L}$$

$$\times Z(\ell_{c}J_{1}\ell_{c'},J_{2};s_{c}L)Z(\ell_{d}J_{1}\ell_{d'},J_{2};s_{d}L)$$

$$Z(\ell_{1}J_{1}\ell_{2}J_{2};sL) = \sqrt{(2\ell_{1}+1)(2\ell_{2}+1)(2J_{1}+1)(2J_{2}+1)} \times (\ell_{1}\ell_{2}00|L0) \times W(\ell_{1}J_{1}\ell_{2}J_{2},sL)$$

and where  $l_c$  and  $s_c$  are the orbital angular momentum and channel spin in channel c and the Z-coefficients are products of one Clebsch-Gordon coefficient and one Racah coefficient W. The angle integrated cross section is

$$\sigma_{cd} = \pi \lambda^2 |\delta_{cd} - S_{cd}|^2$$
<sup>(2)</sup>

and the total cross section is

$$\sigma_{c}^{\text{tot}} = 2\pi \chi^{2} (1 - \text{ReS}_{cc})$$
(3)

In order to treat the energy variations of these cross sections statistically, we must give a statistical description of the energy variations of the S-matrix elements S<sub>cd</sub>. The simplest and most important statistical property of S is its energy average  $\overline{S}$ . Energy averaging does not affect the symmetry property, but it does destroy unitarity, and thereby flux conservation. Averaging cannot create new flux, it can only "absorb" flux into the "compound nucleus" so that the re-emission of this absorbed flux is not described by  $\overline{S}$ . Therefore  $\overline{S}$  must be "less than unitary", which means that the transmission coefficients

$$T_{c} = 1 - \sum_{d} |\overline{S}_{cd}|^{2}$$
must satisfy
$$0 \leq T_{c} \leq 1$$
(5)

where the lower limit implies unitarity of  $\overline{S}$ , and therefore an energy independent S, and the upper limit implies complete absorption of all incoming flux into the compound system. The transmission coefficient  $T_c$  represents the compound nucleus "absorption" cross section in units of  $\pi \chi^2$ .

(5)

The cross sections obtained by substituting  $\overline{S}$  in place of S in Eqs. (1)-(3) are referred to as "direct" cross sections and the direct elastic scattering cross section is called the "shape elastic" cross section. To obtain the complete average cross section  $\overline{\sigma}_{cd},$  the direct cross section must be complemented with the average compound nucleus cross section  $\sigma_{cd}^{fl}$  (also called the fluctuation cross section) which arises from the re-emission into channel d of the absorbed flux  $T_c$ .

The calculation of this average compound nucleus cross section is the principal object of the statistical theory that is of interest to nuclear power applications.

The average S-matrix  $\overline{S}$  is obtained from the optical model by solving the Schrödinger equation with a complex potential interaction between the neutron or other scattered particle and the residual nucleus [1]. The real part of this potential produces shape elastic scattering and the imaginary part is responsible for the compound nucleus absorption. If the optical model Hamiltonian contains also interaction potentials between particles in different reaction channels, then we have a coupled channels optical model with non-vanishing off-diagonal elements of  $\overline{S}$  and with nonvanishing direct reaction cross sections between these channels [2]. Optical and coupled channel models are discussed in greater detail in paper RP5. Among recent developments in the statistical theory is the discussion of the effects of such direct reaction cross sections upon competing compound nucleus cross sections [3,4,5].

The compound nucleus or fluctuation cross section arises from the fluctuating part of the S-matrix

$$S^{f\ell} = S - \overline{S}$$
 (6)

in the following way

$$\sigma_{cd}^{f\ell} = \overline{\sigma}_{cd} - \sigma_{cd}^{direct} = \pi \chi^2 \frac{|S_{cd}^{f\ell}|^2}{|S_{cd}^{f\ell}|^2}$$
(7)

where the superposed bar denotes an energy average. The differential fluctuation cross section is

$$\frac{d\sigma_{cd}^{f\ell}(\Theta)}{d\Omega} = \sum_{L} P_{L}(\cos\Theta) \sum_{c'd'} f_{Lcc'dd'} \operatorname{ReS}_{cc'}^{f\ell} S_{dd'}^{f\ell*}$$
(8)

The simplest assumption leading to expressions for the fluctuation cross section considers that "the average compound nucleus" behaves like a single state of the nuclear system which emits particles into the various reaction channels in the same proportions as it absorbs them. This assumption immediately leads to the well-known Hauser-Feshbach formula for the compound nucleus cross section [6,7].

$$\sigma_{cd}^{\text{H.F.}} = \pi \chi^2 T_c T_d / \sum_e T_e$$
(9)

where the sum in the denominator is taken over all open channels. Adding the assumption that the average of products of different S-matrix elements vanishes, we obtain the differential Hauser-Feshbach formula for the compound nucleus cross section from Eq. (8) and

$$\operatorname{ReS}_{cc}^{f\ell}, \operatorname{S}_{dd'}^{f\ell*} = \left[ \delta_{cd} \delta_{c'd'} + (1 - \delta_{cc'}) \delta_{cd'} \delta_{c'd} \right] \operatorname{T}_{c} \operatorname{T}_{c'} / \sum_{e} \operatorname{T}_{e} \quad (10)$$

In the usual Optical Model with spin-orbit coupling the channel transmission coefficients  $T_c$  depend upon the channel orbital angular momentum  $l_c$  and the total projectile angular momentum  $\vec{J}_c = \vec{l}_c + \vec{s}_c$  (vector addition), where  $s_c$  is the projectile spin ( $\frac{1}{2}$  in the case of nucleons). With this dependence, Goldman and Lubitz have derived the following formula for the differential compound nucleus cross section for spin  $\frac{1}{2}$  particles [8].

$$\frac{d\sigma_{cd}^{\text{H.F.}}(\Theta)}{d\Omega} = \frac{\chi_{c}^{2}(-1)^{\text{I}}c^{-\text{I}}d}{8(2\text{I}_{c}^{+1})} \sum \frac{T_{c}T_{d}}{T_{e}} P_{L}(\cos\Theta)$$
(10a)  
(2J+1)<sup>2</sup>(2j<sub>c</sub>+1)(2j<sub>d</sub>+1)(j<sub>c</sub><sup>1</sup>zj<sub>c</sub>-<sup>1</sup>z|L0)(j<sub>d</sub><sup>1</sup>zj<sub>d</sub>-<sup>1</sup>z|L0)  
W(Jj<sub>c</sub>Jj<sub>c</sub>; I<sub>c</sub>L)W(Jj<sub>d</sub>Jj<sub>d</sub>;I<sub>d</sub>L)

where the summation is over all  $J_{j_c}, j_d, \ell_c, \ell_d$ , and all even L, and where  $I_c$  and  $I_d$  are the target and residual nucleus spins in channels c and d.

The angle integrated cross section averaged over all initial angular quantum numbers and summed over all final angular quantum numbers is then

$$\sigma_{[cd]}^{H.F.} = \pi \chi^2 \sum_{J} \frac{2J+1}{2(2I_c+1)} \frac{T_c T_d}{\sum_{e} T_e}$$
(9a)

where the summation extends also over all  $j_c, l_c, j_d, l_d$ , consistent with total angular momentum J. In both Eqs. (9a) and (10a) the channels e must have total angular momentum J and the same parity as channels c and d. We will henceforth omit the averaging and summation over angular momenta and discuss the individual channel cross sections as in Eq. (9).

The following three sections review the main features of statistical theories and how their predictions of the fluctuation cross section agree or differ from the Hauser-Feshbach formula. The final section deals with situations in which the residual nuclear states have a continuous spectrum or are treated as such.

# 2. ISOLATED RESONANCES

At low neutron energies, the energy dependences of neutron cross sections are well known to arise from sequences of well isolated Breit-Wigner resonances [9]. This behavior is described by an S-matrix which has the form [10]

$$S_{cd} = e^{-i(\phi_c + \phi_d)} \left( \delta_{cd} - i \sum_{\mu} \frac{f_{\mu c} f_{\mu d}}{E - E_{\mu} + \frac{1}{2} i \Gamma_{\mu}} \right)$$
(11)

where the total widths  $\Gamma_{\!\mu}$  are related to the partial widths  $\Gamma_{\!\mu c}$  and the real width amplitudes f\_{\mu c} by

$$\Gamma_{\mu c} = f_{\mu c}^2 , \ \Gamma_{\mu} = \sum_{c} \Gamma_{\mu c}$$
(12)

and where all widths  $\Gamma_{\mu}$  are small compared to the spacings between resonance energies  $\text{E}_{\mu}$  .

Averaging Eq. (11) over energy, we obtain the optical model Smatrix elements

$$\overline{S}_{cd} = e^{-i(\phi_c + \phi_d)} (\delta_{cd} - \pi \langle f_{\mu c} f_{\mu d} \rangle_{\mu} / \mathcal{D})$$
(13)

where D is the mean spacing of the  $E_{\mu}$  and the bracket  $\langle \rangle_{\mu}$  refers to an average with respect to the resonance index  $\mu$ , taken over all resonances within the averaging interval. We see immediately that in the absence of direct reactions when  $\overline{S}_{cd}$  vanishes for  $c\neq d$ ,  $\langle f_{\mu c} f_{\mu d} \rangle_{\mu}$  must also vanish, and vice versa. We shall assume here that  $\overline{S}$  is diagonal and return to the case of direct reactions in Section 4. Then we have

$$\overline{S}_{cd} = \delta_{cd} e^{2i\phi} c (1 - i\pi \langle \Gamma_{\mu c} \rangle_{\mu} / D)$$
(14)

which leads to

$$T_{c} = 1 - |\overline{S}_{cc}|^{2} = \frac{2\pi \langle \Gamma_{\mu c} \rangle_{\mu}}{\mathcal{D}} - \frac{\pi^{2} \langle \Gamma_{\mu c} \rangle^{2}}{\mathcal{D}^{2}}$$
(15)

where we will ignore the second term in the limit of small  $\langle \Gamma_{\mu c} \rangle / D$ , that is in the limit of small transmission coefficients.

In this same limit the fluctuation cross section is easily calculated from the S-matrix (11) with the assumption that  $\overline{S}$  is diagonal, and one obtains

$$\sigma_{cd}^{f\ell} = \frac{2\pi^2 \chi^2}{D} \left\langle \frac{\Gamma_{\mu c} \Gamma_{\mu d}}{\Gamma_{\mu}} \right\rangle_{\mu}$$
(16)

which, on omitting the second term in Eq. (15) becomes [11-14]

$$\sigma_{cd}^{f\ell} = \pi \chi_c^2 \sigma_{cd}^{H,F} F_{cd}$$
(17a)

where

1

$$F_{cd} \equiv \left\langle \frac{\Gamma_{\mu c} \Gamma_{\mu d}}{\Gamma_{\mu}} \right\rangle_{\mu} / \frac{\left\langle \Gamma_{\mu c} \right\rangle_{\mu} \left\langle \Gamma_{\mu d} \right\rangle_{\mu}}{\left\langle \Gamma_{\mu} \right\rangle_{\mu}}$$
$$= (1+2\frac{\delta_{cd}}{\nu_{d}}) \int_{0}^{\infty} dt \prod_{f} (1 + \frac{2tT_{f}}{\nu_{f} \sum_{q} T_{g}})^{-(\frac{1}{2}+\delta_{f}c^{+\delta}fd^{+})}$$
(17b)

In this integral evaluation of the width fluctuation correction  $F_{cd}$  to the Hauser Feshbach formula, it is assumed that the distribution of values of the partial widths  $\Gamma_{\mu c}$  for each channel c is given by the chi-squared distribution law with  $v_c$  degrees of freedom, which is defined for any positive real v by the frequency function

$$F_{v}(x) = x \left(\frac{v}{2} - 1\right)_{e} - \frac{x}{2} / \left(2^{2} \Gamma(\frac{v}{2})\right)$$
(18)

Tepel et al. [15] found a formula which yields a very good approximation to the width fluctuation corrected Hauser Feshbach formula of Eqs. (17) in most instances, but does not require the integration of Eq. (17b). According to these authors

$$\sigma_{cd}^{f\ell} \stackrel{\sim}{\sim} \pi \chi_{c}^{2} (Y_{c}Y_{d} + 2\delta_{cd}Y_{d}^{2}/\nu_{d}) / \sum_{e} Y_{e}$$
(19a)

where

$$Y_{c} = \frac{T_{c}}{1 + \frac{2}{v_{c}} \frac{T_{c}}{\sum_{e} T_{e}}}$$
(19b)

Clearly, in the case of isolated resonances with no direct reactions, the only information which we need in order to evaluate the fluctuation cross sections is the optical model transmission coefficients and the partial width distribution laws for all open channels. There is considerable theoretical as well as experimental evidence that in this isolated resonance limit the  $f_{\mu c}$  of Eq. (11) are normally distributed with zero means. It follows from this that the  $\Gamma_{\rm uc}$  are distributed according to the chi-squared distribution with one degree of freedom (the Porter-Thomas distribution) for any "channel" c which is specified by a single complete set of quantum numbers describing the channel angular momenta and the state of the residual nucleus [16-17]. This is the case for neutron and proton partial widths in channels having a specified orbital and total angular momentum and a specified residual nuclear level. Any "channel" that is specified by n independent quantum channels all having the same average partial width, is distributed according to a chi-squared distribution with n degrees of freedom. Thus "capture" generally encompasses a large number of independent gamma ray transitions to various low lying levels of the compound nucleus, and therefore the capture width has a very narrow distribution corresponding to a large degree of freedom (see paper RP3). Fission, which often proceeds by one of several independent processes, gives rise to fission widths which have generally between two and three degrees of freedom, depending on isotope and energy. Fission will be discussed in paper RP7.

The effect of the width fluctuation correction is to increase the compound elastic fluctuation cross section and to decrease non-elastic cross sections correspondingly. The effect of this correction is particularly pronounced for the inelastic scattering to the first excited state of an even A nucleus, which can be reduced by almost a factor of  $\frac{1}{2}$  compared to Hauser-Feshbach. Correspondingly the compound elastic cross-section is enhanced by almost 50% compared to Hauser-Feshbach. When many channels are open, the effect on each inelastic cross section becomes less pronounced, but the compound elastic effect increases to a possible maximum enhancement by a factor of 3. Some typical magnitudes of the width fluctuation correction are shown in the

graphs of <u>Fig. 1</u> and a typical example of the effect upon inelastic scattering to the first excited state in even A nuclei is shown in <u>Fig. 2.</u>

There are, of course, other interesting statistical properties that affect the details of the energy variations of the cross sections, such as the behavior of the level densities and the distribution of level spacings. The level densities will be reviewed in paper RP4. Level spacing distribution laws have been very intensively studied by a number of authors [14,17]. But this subject is of very limited interest to nuclear power applications.

In computing elastic and non-elastic neutron scattering cross sections, it is important, particularly at low energies, to include the contribution  $T_{\gamma} = 2\pi\Gamma_{\gamma}/D$  of the capture channels to the transmission factor sum in the Hauser-Feshbach cross section in Eq. (17), as is done in the computer program NEARREX [18]. The effect of the capture channels on the width fluctuation correction (17) can be taken into account by an additional factor of exp  $[-tT_{\gamma}/\sum_{g} T_{g}]$  in the integral [13]. This treatment assumes that the capture widths do not fluctuate. Computer programs for the calculation of average cross sections by the width-fluctuation corrected Hauser-Feshbach formula include NEARREX [18], ALTE [19], and STAX 2 [20].

# 3. INTERFERING RESONANCES

As we have seen in Eq.(15), the results of the previous section break down as soon as  $T_c$  for some channel is no longer very small, as will happen for low angular momentum neutron channels at quite moderate energies of typically some tens of kilovolts. Then  $\langle \Gamma_{\mu} \rangle_{\mu} / D$  is no longer very small and consequently at some energies more than one term in the resonance sum of Eq.(11) will contribute significantly to S. At such energies the expression (11) is not unitary and it can be shown that it is in fact impossible to make Eq.(11) unitary at all such energies with real parameters  $f_{\mu c}$ .

In order to retain unitarity, Eq.(11) must be modified to read [10,21,22]

$$S_{cd} = S_{cd}^{b} - i \sum_{\mu} \frac{g_{\mu c} g_{\mu d}}{E - E_{\mu} + \frac{1}{2} i \Gamma_{\mu}}$$
 (20)
where the  $S_{cd}^{b}$  and the  $g_{\mu c}$  are complex parameters that are only slowly energy dependent, and that satisfy complicated and not yet fully understood relations in place of Eq. (12).

Two known relations that the parameters of Eq. (20) must satisfy in the case of diagonal  $\overline{S}$  are, first of all [23]

$$2\pi \left\langle g_{\mu c}^{2} \right\rangle_{\mu} / D = \overline{S}^{*-1} - \overline{S}$$
(21a)

or

$$|2\pi \langle g_{\mu c}^{2} \rangle_{\mu} / D|^{2} = T_{c}^{2} / (1 - T_{c})$$
(21b)

where D is the mean spacing of the  $E_{\mu}$  in (20). Secondly we have the requirement that [24,25]

$$\overline{S}_{cc} = e^{-\pi \langle \Gamma_{\mu c} \rangle_{\mu} / D} , \quad \langle \Gamma_{\mu} \rangle_{\mu} = \sum_{c} \langle \Gamma_{\mu c} \rangle_{\mu}$$
(22a)

or

$$T_{c} = 1 - e^{-2\pi \langle \Gamma_{\mu c} \rangle_{\mu} / D}$$
(22b)

and it follows from (21) and (22) that

$$\pi |\langle g_{\mu c}^{2} \rangle_{\mu} |/D = \sinh(\pi \langle \Gamma_{\mu c} \rangle_{\mu} / D)$$
(23)

which shows that the mean partial width becomes logarithmically infinite as T<sub>c</sub> approaches unity, and that the absolute mean square amplitudes  $g_{\mu c}$  grow exponentially compared to the mean partial widths.

We can again calculate the optical model S-matrix and the fluctuation cross section and obtain [21]

$$\overline{S}_{cd} = S_{cd}^{b} - \pi \langle g_{\mu c} g_{\mu d} \rangle_{\mu} / D$$
(24)

which implies quite generally, that in order for  $\overline{S}$  to have off-diagonal elements, either  $S^b$  or  $\langle g_{\mu} \times g_{\mu} \rangle_{\mu}$  or both must have off-diagonal elements. The possibility that the two terms cancel is effectively excluded. The fluctuation cross section for diagonal  $\overline{S}$  is [21,25]

$$\sigma_{cd}^{f\ell} = \pi \chi^{2} (2\pi/D) \langle |g_{\mu c}|^{2} |g_{\mu d}|^{2} / \Gamma_{\mu} \rangle - M_{cd}$$
(25)

where

$$M_{cd} = \frac{1}{2} \delta_{cd} T_{c}^{2} / (1 - T_{c}) - (2\pi i/D) \left\langle \sum_{\nu \neq \mu} \frac{g_{\nu c} g_{\nu d} g_{\mu c}^{*} g_{\mu d}^{*}}{(E_{\mu} - E_{\nu})^{+\frac{1}{2}} i (\Gamma_{\mu} + \Gamma_{\nu})} \right\rangle_{\mu}$$
(26)

The first term in Eq. (25) looks like Hauser-Feshbach but is difficult to evaluate because we know nothing about the  $|g_{\mu c}|^2$  except that they are proportional to the  $\Gamma_{\mu c}$  independent of channel index [10,21].

$$|g_{\mu c}|^2 / \Gamma_{\mu c} = N_{\mu}^2 \frac{1}{2}$$
 (27)

This fact permits us to define the quantities [21]

$$\Theta_{\mu c} = (2\pi/D) N_{\mu}^{2} \Gamma_{\mu c} , \Theta_{\mu} = \sum_{c} \Theta_{\mu c}$$
(28)

from which

$$\sigma_{cd}^{f\ell} = \pi \chi^{2} \left( \left\langle \Theta_{\mu c} \Theta_{\mu d} / \Theta_{\mu} \right\rangle - M_{cd} \right)$$
(29)

and

$$T_{c} = \langle \Theta_{\mu c} \rangle_{\mu} - \sum_{d} M_{cd}$$
(30)

The evaluation of the first term of Eq. (29) is complicated by the fact that it can be shown that there exist correlations between the  $\Theta_{\mu c}$  for different channels [26] even in the absence of direct reactions, and these correlations make the evaluation much more difficult than in the case of Eq. (16) where the  $\Gamma_{\mu c}$  were not correlated for different channels. Also the evaluation of the second term in Eq. (26) depends on a knowledge of possible resonance-resonance correlations of the  $g_{\mu c}$  [27].

It has been shown that in a certain class of cases, the effect of the channel-channel correlations of the  $\Theta_{\mu c}$  just cancels the contribution of M [26]. Assuming this M-cancellation to be generally valid one arrives at a formula for the fluctuation cross section that is identical to the width fluctuation corrected Hauser-Feshbach formula (17). The only difference is that now we do not know the values of the fluctuation indices  $v_c$  for the various channels as we did in the case of isolated resonances. From general theoretical considerations one deduces that for each independent channel the value of  $v_c$  rises from 1 towards a limiting value of 2 as  $\langle \Gamma \rangle / D$  increases. From certain numerical studies Tepel et al. [15] have deduced an empirical expression for  $v_c$  as a function of  $T_c$ 

$$v_{\rm c} = 1 + T_{\rm c}^{\rm L_2}$$
 (31)

Other more complicated functional relationships have been proposed elsewhere [4]. However almost certainly the value of  $v_c$  does not only depend on  $T_c$  but also on the transmission coefficients of all competing channels. If channels with large transmission coefficients compete with a channel c having a small  $T_c$ , the value of  $v_c$  will be larger than indicated by Eq. (31) [26]. More work is required in this area.

It is important to note that the M-cancellation principle replaces an earlier attempt to take into account the second term in Eq. (30) by modifying the definition of  $T_c$ , using parameter  $Q_c$  [18,21, 25].

There exist two other methods for treating the fluctuation cross section which are so far applicable only to the limit of very large  $\langle \Gamma \rangle / D$ . They may therefore not be usable in many situations of interest to nuclear power applications. The first of these is the treatment of Kawai, Kerman and McVoy which is based upon a representation of the S-matrix that looks very much like Eq. (20), but whose parameters are chosen in such a way that S is not unitary at all energies [3]. The resulting fluctuation cross section formula, which does not involve the difficult expression M in Eq. (24) yields virtually identical results to those obtained from the M-cancellation procedure in the limit of large  $\Gamma / D$  if all channel fluctuation indices are chosen to have the value  $v_{c} = 2$ . We shall return to this formula in the next section.

There is also a new and entirely different method due to Agassi and Weidenmüller which is based upon the doorway state description of the nuclear reaction mechanism (see paper RP6), and which yields correction terms to the Hauser-Feshbach formula in the limit of large  $\langle \Gamma \rangle /D$  [28].

# 4. DIREGT REACTION EFFECTS

As we saw in Eq. (13), one obvious effect of direct reactions is

that they can produce correlations between the partial widths of different channels. (Actually, Eq. (11) must be modified to permit also nonresonant off-diagonal terms if direct reactions are present.) Correlations in partial widths of different channels must be expected to produce enhanced fluctuation cross sections between these channels. The reason for this is the same as the reason for the width-fluctuation enhancement of the elastic fluctuation cross section, Eq.(17), which arises from the complete correlation of entrance and exit channel widths in the elastic case, where the two are identical. Thus the effect of direct reactions upon average compound nucleus cross sections is basically an aspect of the width fluctuation correction. In the case of isolated resonances the direct effect can be calculated in this way [29.30]. However the most general and useful method is the use of the Engelbrecht-Weidenmüller transformation [31] which is a linear transformation of the reaction channels that results in a transformed unitary S-matrix with a diagonal average.

This transformation is specified by the unitary matrix U that diagonalizes the Hermitean penetration matrix P of Satchler [32]

$$P = 1 - \overline{S} \overline{S}^*$$
(32)

$$P'= UPU^{-1}$$
 is diagonal, (33)

where  $U^{-1} = U^{\dagger}$  .

It follows then that

$$S' = USU$$
 (34)

is unitary, where  $\check{\mathcal{U}}$  is the transpose of U, and  $\overset{\sim}{\scriptstyle \mathcal{V}}$ 

$$\overline{S}' = U\overline{S}U$$
 is diagonal (35)

Arguments have also been given that S' has the same statistical properties as a physical S-matrix with diagonal average [4]. For the case of only two directly coupled channels, the transformation U is easily written down explicitly [5]. Writing

$$\overline{S} = \begin{pmatrix} f_1 e^{i\Theta_1} & f_3 e^{i\Theta_3} \\ f_3 e^{i\Theta_3} & f_2 e^{i\Theta_2} \end{pmatrix}$$
(36)

and  $U = \begin{pmatrix} \cos\beta & -\sin\beta \\ \sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix}$  (37)

we find that

$$\tan 2\alpha = \frac{f_2 \sin \Theta_{23} - f_1 \sin \Theta_{13}}{f_2 \cos \Theta_{23} + f_1 \cos \Theta_{13}}$$
$$\tan 2\beta = \frac{2f_3}{f_2 \cos (\Theta_{23} - \alpha) - f_1 \cos (\Theta_{23} - \alpha)}$$
(38)

where  $\Theta_{13} = \Theta_1 - \Theta_3$ ,  $\Theta_{23} = \Theta_2 - \Theta_3$ .

For three or more coupled channels the direct effect will in general not be very significant as we shall see. In such cases numerical diagonalization of P is required.

With the help of the Engelbrecht-Weidenmüller transformation the fluctuation cross section can be expressed entirely in terms of the elements of the transformation matrix U, and certain averages of the transformed S-matrix S'. Two types of such averages occur. The first is of the form  $|S_{cd}^{ifl}|^2$ , which is just the fluctuation cross section (7) in the transformed channel space and can be evaluated by the width fluctuation corrected Hauser-Feshbach formula as described in Sections II or III. For this one requires the transmission coefficients in the transformed channel space, which are just the diagonal values of the transformed penetration matrix P'. One also requires the fluctuation parameters  $v_c^i$  (Eq. 31) for each of the transformed channels in order to compute the width fluctuation correction factors  $F_{cd}^i$ . Then

$$\sigma_{cd}^{if\ell} = \pi \chi_{c}^{2} \frac{|S_{cd}^{if\ell}|^{2}}{|S_{cd}^{if\ell}|^{2}}$$

$$= \pi \chi_{c}^{2} (P_{cc}^{i}P_{dd}^{i}/trP^{i}) F_{cd}^{i}.$$
(39)

In addition there also occur averages of another type, which can be estimated by means of the M-cancellation procedure as follows

$$\pi \tilde{\chi}_{c}^{2} \frac{\overline{S_{cc}^{\dagger f \ell} S_{dd}^{\dagger f \ell \star}}}{S_{cc}^{\dagger} S_{dd}^{\dagger \ell \star}} = \sqrt{\frac{2 - v_{c}^{\dagger}}{v_{c}^{\dagger}} \cdot \frac{2 - v_{d}^{\dagger}}{v_{d}^{\dagger}}} \sigma_{cd}^{\dagger f \ell}$$
(40)

Using Eqs. (35), (39), (40) one obtains for the fluctuation cross section in the presence of direct reactions [5]

$$\sigma_{cd}^{f\ell} = \sum_{e} |U_{ec}|^{2} |U_{ed}|^{2} \sigma_{ee}^{if\ell} + \sum_{f\neq e} \left[ \frac{|U_{ec}|^{*} |U_{ed}|^{*} |U_{ec}|^{*} |U_{ec$$

A very similar formula that yields almost entirely equivalent results, but is a little more complicated to evaluate, has been given by Hofmann et al. [4]. The formula of Kawai, Kerman and McVoy [3] yields results equivalent to Eq. (41) <u>only</u> in the limit of large  $\langle \Gamma \rangle$ /D when all  $\nu_c$  are equal to 2. Then this formula reads

$$\sigma_{cd}^{f\ell} = \chi_{cc} \chi_{dd} + \chi_{cd} \chi_{dc}, \quad \langle \Gamma \rangle >> D$$
(42)

$$P_{cd} = \sum_{e} (X_{cd} X_{ee} + X_{ce} X_{ed})$$
(43)

Here Eq. (43) must first be solved for X by numerical iteration and then substituted into Eq. (42).

Qualitatively we see from Eq. (41) that the enhancement of the fluctuation cross section due to direct reactions is at most equal to the width-fluctuation enhancement of the transformed elastic fluctuation cross section  $\sigma_{ee}^{ifl}$ . This enhancement amounts at most to a factor of 1 +  $2/v_e^{\prime}$  and will in practice almost always be less than a factor of 2. The maximum enhancement is achieved when only two channels are directly coupled to one another and det P = 0. In that case the transmission coefficients for one of the two transformed channels vanishes, and therefore there is only one independently fluctuating transformed channel. As a result, the fluctuations in the two coupled physical channels are completely correlated, just as in the case of compound elastic scattering. The case det P = 0 is called the causality limit because causality considerations are violated when det P is negative [5]. Eq. (41) predicts that enhancements due to direct reactions are appreciable only quite close to the causality limit when that limit is not identical to the unitarity limit trP=0. Ordinarily large enhancements will occur only when the rank of P is no greater than 2. Fig. 3 shows the enhancement due to direct reactions as computed by

means of Eq. (40) for two types of  $\overline{S}$  matrices. In one of these (upper right) the causality limit coincides with the unitarity limit, and there is no appreciable enhancement. In the other case the causality limit is not equal to the unitarity limit and enhancements close to a factor of 2 occur.

The validity of the results of Eq. (41) have been confirmed by computer averaging of computer generated statistical model cross sections [5]. Such calculations have also been used to confirm the M-cancellation principle for a wide variety of  $\overline{S}$  matrices [26].

# 5. CONTINUOUS CHANNELS

With increasing neutron energy the number of open exit channels increases rapidly until it is either impossible or undesirable to enumerate all such channels and discuss their cross sections in detail. It then becomes necessary to discuss the differential cross section for transitions to channels of a given type (e.g., neutron or protons, etc.) leaving the residual nucleus with an excitation energy within a differential interval at  $E_d$ .

$$\frac{d\sigma_{cd}^{fl}(cont.)}{dE_{d}} = \sigma_{cd}^{fl}(discr.) \rho_{d}(E_{d})$$
(44)

where  $\sigma_{cd}^{fl}(\text{discr.})$  is the cross section for excitation of a discrete channel with residual nuclear excitation  $E_d$ , and  $\rho_d(E_d)$  is the level density at excitation  $E_d$  of the residual nucleus in channel d for states having spin and parity specified by the channel index d. We refer again to paper RP4 for a detailed discussion of level densities.

If the dependence of  $\rho_d$  upon the relevant residual spins  $I_d$  is given by the factor (2 $I_d$ +1), then it can be shown that the fluctuation cross section (44) summed over  $I_d$  is isotropic. Though this spin dependence of  $\rho_d$  is not correct, the anisotropies of fluctuation cross sections at such high energies are expected to be small and can often be ignored.

Also, in the presence of large numbers of competing channels, the width fluctuation correction and direct effect upon non-elastic fluctuation cross sections becomes negligible. On the other hand for  $\langle T \rangle >>D$  we expect an elastic width fluctuation correction factor of 2, so that in the present domain we expect that

$$\sigma_{cd}(discr.) \cong (1 + \delta_{cd}) \sigma_{cd}^{H.F.}$$
, (45)

where again, the channel indices c and d carry all relevant energy and angular momentum quantum numbers.

The transmission factor sum  $\sum_{e} T_{e}$  which occurs in the denominator of  $\sigma_{cd}^{\text{H.F.}}$ , Eq. (9), must also be evaluated statistically

$$\sum_{e} T_{e} = \sum_{e} \int_{0}^{E_{e}(\max)} T_{e}(E_{e})\rho_{e}(E_{e})dE_{e}$$
(46)

which involves the level densities for the residual nuclei in all competing channels. Again, if  $\rho_e$  depends on the residual nucleus spin through a factor (21<sub>e</sub>+1), then the transmission sum (46) is given by [33]

$$\sum_{e} T_{e} = (2J+1)G/\pi$$
 (46a)

where J is the total angular momentum and G depends only upon excitation energy of the compound nucleus.

Another empirical method for determining the transmission factor sum makes use of the relation [34]

$$\sum_{e} T_{e} \stackrel{\simeq}{=} 2\pi \Gamma^{corr} / \rho \tag{47}$$

where  $\Gamma^{\rm corr}$  is the correlation width and  $\rho$  is the compound nucleus level density for states of the same total angular momentum and parity as the channels e that are summed over. The correlation width can under some circumstances be estimated from fluctuation experiments [35]. The validity of the relation (47) was recently confirmed by numerical studies [26]. Comparison of Eqs. (22b) and (47) shows that the correlation width of Eq. (47) is not the same as the average of the widths  $\langle \Gamma_{\rm u} \rangle_{\rm u}$  of Eq. (20).

Difficulties remain in the reliable treatment of compound nucleus cross sections at high energies. These are caused by a number of different circumstances. First, there is the uncertainty regarding the effects of gamma ray transitions between highly excited compound nuclear states in softening the spectrum of emitted neutrons and protons. Secondly, there are empirical results which disagree with the shapes of the particle spectra predicted by the above statistical picture. This effect has been treated with considerable success by means of the pre-equilibrium models which will be discussed in paper RP6 [36].

Finally, at neutron energies exceeding 10 to 20 MeV, residual nuclear levels become unstable and emit secondary particles which further add to the particle flux generated by the reaction. From a theoretical viewpoint, such physically continuous channels pose a threeor more body problem in the channel portion of configuration space, not just in the compound nucleus. While theoretical methods exist now for treating three-body problems [37], they are complicated and time-consuming and have not yet been applied to neutron induced reactions in heavy nuclei. It is therefore generally assumed that above the threshold for three body breakup, the breakup proceeds sequentially. That is, in addition to the particle spectrum produced according to Eq. (44), there are additional particles produced by the breakup of the residual nuclei in each channel d which is given by

$$\int_{0}^{E_{d}(\max)} dE_{d}\sigma_{cd}^{f\ell}(discr.)\rho_{d}(E_{d}) T_{d},\rho_{d},(E_{d},)/\sum_{e'}T_{e'}$$
(48)

where the channels d' are decay channels of the residual nucleus of channel d, considered as a new compound system, etc.

When level densities are computed from the model of the nucleus which pictures it as a gas of fermions, characterized by a temperature parameter, the particle spectra produced according to Eqs. (44), (48), etc., are called evaporation spectra. Probably in most instances, the doorway state models involving precompound or pre-equilibrium decay (see paper RP6) give a better account of these spectra.

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# FIGURE CAPTIONS

- Fig. 1. Some non-elastic width fluctuation correction factors for two channels (x and y) having v=1 (Porter-Thomas) and one channel (Z) having v=∞ (exponential, equivalent to large numbers of competing channels ).
- Fig. 2. A typical example of the effect of the width fluctuation correction on the excitation cross section of the first  $2^+$  state in an even target nucleus. Shown are the Hauser-Feshbach prediction and the width fluctuation corrected predictions for v=l and v=2 for the 845 keV level in iron. Optical potential and data points are from Ref. [38]. (Neutron time-of-flight spectroscopy.) The data curve is from Ref. [39] (gamma ray spectroscopy.)
- Fig. 3. Predicted enhancements of compound non-elastic cross sections due to competition with direct reactions for two classes of coupled channel S-matrices (From Ref. [5])









Fig. 2.

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Fig. 3.

Review Paper No. 3

RADIATIVE CAPTURE OF 5-20 MeV NEUTRONS

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### ABSTRACT

The paper reviews the refinements introduced in the direct-semidirect model to attain greater reliability in calculations of  $(n,\gamma)$  cross sections for high-energy neutrons. Outlines of different reaction mechanisms are given and the results of theory are compared with available experimental data. The possibility of using the direct-semidirect model for calculation of  $\gamma$ -ray spectra and cross sections for the production of 8-20 MeV photons is discussed.

#### 1. INTRODUCTION

Increasing interest in fast fission reactors as well as in fusion reactors makes an attempt to provide data on radiative capture of fast neutrons necessary. In particular, one requires a detailed knowledge of the photoproduction cross sections and gamma-ray spectra for neutron energies up to perhaps 20 MeV. In view of the experimental difficulties it is necessary to proceed at one and the same time with both measurements and calculations in order to provide indications as to the required data. The present review deals with radiative capture of 5-20 MeV neutrons by heavy and medium-mass target nuclei (A>40).

Essentially three different mechanisms (compound nucleus, direct and semidirect capture) have been proposed in an attempt to explain the experimental data of the  $(n,\gamma)$  reaction in the energy region considered. The compound-nucleus theory does not give an adequate account of the measured data, especially in heavy nuclei. The direct capture process attenuates the disagreement, still predicting cross sections sometimes an order of magnitude less than the measured ones. Several analyses indicate that, taken together,



Fig.1. Energy spectrum of gamma-rays from 14.2 MeV neutron bombardment of  $^{93}$ Nb for  $\Theta$ =125° (reproduced from Ref.[1] ).

the direct and semidirect processes are adequate to explain the experimental data.  $\langle$ 

The refinements introduced in the semidirect model to attain greater reliability in calculations are here briefly reviewed, predictions of theory are compared with experimental data and the available computer codes are referred to. The review emphasizes the possibility of using the direct-semi direct model for satisfying requests as to  $(n,\gamma)$  cross sections, gamma-ray spectra and photoproduction cross sections.

Experimental data and calculations of gamma-ray production cross sections are usually limited to photons with energy up to about 8 MeV. This main part of gamma-ray production from reactions induced by 5-20 MeV neutrons is essentially due to nonelastic reactions, while for producing higher energy photons radiative capture is probably the dominant mechanism. For 8-20 MeV photons, model calculations of a statistical nature become unreliable and experimental uncertainties reach one or two orders of magnitude, as can be seen, for example, from <u>Fig. 1</u> reproduced from the review paper by Young [1]. Usually the intensity of 8-20 MeV gamma-rays is relatively low, but, because of their high penetrability information on their production cross sections may be useful for application purposes. Therefore use of calculations based on the direct-semidirect model to fill the gaps in experimental data is here discussed.

#### 2. STATUS OF THE THEORY

# 2.1. Outlines of the capture mechanisms

The radiative capture of 5-20 MeV neutrons has been described by three reaction mechanisms which may be outlined as follows.

The first process proposed was the capture of a neutron through the formation of a compound system with a relatively long life-time. According

to this model, an incident neutron entering the target nucleus forms a compound nucleus in an excited state. The excitation energy, the sum of neutron kinetic and separation energies, is transmitted and shared among many nucleons. Then radiative transitions from this state to the lower ones take place until the ground state is reached, as shown in <u>Fig. 2a</u>). The decay can be considered as a statistical process and the cross section, as well as the  $\gamma$ -ray spectrum emitted in decay, can be calculated by statistical methods. In this spectrum low-energy gamma rays are dominant.

The direct capture model [2] considers that the incident neutron, during its movement in the mean nuclear potential field of the target nucleus, emits a  $\gamma$ -ray undergoing a direct transition to an unoccupied particle bound state, as shown in Fig. 2b).

state, as shown in <u>Fig. 2b</u>). In the semidirect [3] or equivalent collective model [4] the capture proceeds through intermediate states. In the collective picture the target nucleus may have shape oscillations and an incident nucleon experiences a slightly deformed potential. The interaction of the nucleon with the nucleus through such a potential can excite collective modes of the target. In the capture process the nucleon is scattered into an empty particle bound state and the nucleus is excited to its giant dipole state. The latter then decays emitting a  $\gamma$ -ray. A schematic picture of this mechanism is given in <u>Fig. 2c</u>). According to the direct or semidirect model the capture of neutrons leading to bound final states by the emission of one photon is favoured. Therefore a dominance of high-energy photons in the spectra is expected.

As is well known, the compound-nucleus theory fails to explain both radiative capture cross sections for neutron energies greater than 5-10 MeV, and the shape of observed gamma-ray spectra. It should be noted however that a contribution by this mechanism may be useful in fully explaining experimen tal data, especially in the 5-10 MeV neutron-energy region. In what follows the interest focuses on the direct and semidirect models, which together have given reasonable agreement with experimental data.

## 2.2. The direct-semidirect model

It had been clear since the appearance of the semidirect model that this mechanism could explain the energy dependence and the order of magnitude of the  $(n,\gamma)$  cross sections. This encouraged efforts to develop and refine the models in order to attain more detailed agreement between theory and experiment.

A first step was achieved [5] by introducing spin-orbit effects in collective capture. Subsequently, the direct [2] and collective [4] models were considered together and the importance of the interference between these two processes was shown [6].

Even with these refinements, however, in many cases the agreement in magnitude between theory and experiment was reached by using questionable values for some of the input parameters. This indicated that some further improvement should be introduced into the substantially satisfactory semidirect theory. In the last four years efforts have mainly been directed towards modifying the form of the particle-vibration coupling through which a target collective state is excited and the incident neutron is captured to a bound state.

In the present formulation the direct-semidirect radiative capture cross section can be expressed in a general form as

$$\sigma(\mathbf{n},\gamma) = \frac{\pi}{\mathbf{k'}^2} \sum_{\ell j j'} |A_{\ell j j'} + B_{\ell j j'}|^2 , \qquad (1)$$



Fig.2. Schematic picture of different reaction mechanisms for neutron radiative capture.

where k' is the incident wave number while  $A_{jj}$ , and  $B_{jj}$ , explicitly given in Ref.[6] are the direct and semidirect radiative-capture amplitudes for a transition from a given initial state (l'j') to an individual particle bound state (l j). The dominant contribution to the cross section value comes from the semidirect term whose amplitude can be written

$$B_{\ell j j} = F_{\ell j j}, \quad \frac{\int u_{\ell j}(\mathbf{r}) \mathbf{h}(\mathbf{r}) \psi_{\ell' j}(\mathbf{r}) \mathbf{r}^2 d\mathbf{r}}{\varepsilon_{\gamma} - \hbar \omega_1 + \frac{i}{2} \Gamma} \quad . \tag{2}$$

As expression (2) clearly shows, this amplitude is modulated by an energy factor with  $\varepsilon_{\gamma}$  the energy of the emitted  $\gamma$ -ray (equal to the sum of incident and bound state neutron energies) and  $\pi\omega_{\mu}$  and  $\Gamma$  the excitation energy and width of the giant dipole state in the target nucleus.

In order to obtain the semidirect amplitude one has to calculate the integral of expression (2) in which  $u_{gi}(r)$  and  $\psi_{gij}(r)$  are the radial parts of the bound state and incident nucleon wave functions, and h(r) a function proportional to the particle-vibration coupling interaction for excitation of the giant dipole state. The differences in the various formulations of the direct-semidirect model are mainly related to the use of different expressions for h(r).

In the original paper [4] the particle-vibration coupling interaction was given a surface-peaked real form, which can be written as

$$h_{surf}(r) = v_1 \eta(r) = -v_1 \frac{4\pi}{3A} \frac{d\rho(r)}{dr}$$
, (3)

with  $v_1$  the strength of the isospin real term in the optical potential and  $\rho(r)$  the nucleon density.

Comparisons between theory and experiment have been made in a great number of cases by using the surface form (3) of the coupling interaction (see, for example, Refs. [6-21]). It was found that the theory was adequate to account for the shape of the  $\gamma$ -ray spectra observed and the energy depen dence of the  $(n,\gamma)$  cross sections in the giant resonance region. As far as the absolute magnitude of the cross sections was concerned, it appeared, however, that the calculated values were generally smaller than the experimental ones, unless input parameters lying beyond the experimental uncertainty were used. For example, in many cases agreement in magnitude between theory and experiment was reached by using in the calculations a lower value for the width of the dipole state  $\Gamma$  than that obtained from the  $(\gamma,n)$  giant-resonance data, and a value for  $v_1$  (the isospin term in the optical potential) which may be too high.

Subsequently, a real "volume" form was introduced [22] for the coupling interaction between the neutron and the nuclear El mode

$$h_{vol}(r) = v_1 \xi(r) = v_1 \frac{4\pi}{A < r^2 >} r \rho(r) ,$$
 (4)

with  $\langle r^2 \rangle$  the mean-square nuclear radius. It should be noted that in both formulae (3) and (4) the strength of the coupling interaction is given direct ly by the value of  $v_1$  while the form factors  $\eta(r)$  and  $\xi(r)$ , satisfying the normalization condition

$$\int \eta(r) r^{3} dr = \int \xi(r) r^{3} dr = 1 , \qquad (5)$$

determine only the radial dependence of the interaction.

Use of the volume form of the particle-vibration coupling permits one to increase the calculated cross sections by about a factor of 2 or 3, thus giving better agreement with experimental data. An example of such calculations is given in <u>Fig. 3a</u>), which shows a comparison between experimental [18, 23] and theoretical [24] cross sections for the  $^{208}\text{Pb}(n,\gamma)$  reaction. The continuous and dashed curves are calculated with the same set of parameters by using the volume form (4) of the interaction in the former case and the surface form (3) in the latter one. A magnitude enhancement of the cross section, similar to that shown in <u>Fig. 3a</u>), has also been obtained in the other cases considered (see for example Refs. [22, 24-30]).

However, as can be seen from <u>Fig. 3a</u>), a discrepancy between theory and experiment still remained on the low energy side of the giant resonance. The situation was no better when using a mixed surface plus volume form of the coupling [31].

To remove this discrepancy the complex interaction

$$h(r) = v_1 \xi(r) + i w_1 4b \frac{4 < r >}{< r^2 >} \eta(r)$$
(6)

was proposed [32]. Here  $w_1$  is the strength of the imaginary part of the symmetry potential and <u>b</u> the diffuseness parameter.

Inclusion of the imaginary part of the interaction increases the calculated cross section and helps to remove the discrepancy between theory and experiment on the low energy side of the giant resonance. In fact, it was shown in Ref. [6] that a real coupling interaction is responsible for constructive interference between direct and semidirect capture on and above the giant resonance peak and for destructive interference below it. Of course, an opposite sign in the interference term is obtained from an imaginary inter action, thus displacing the cross section peak towards lower energies. Fig. 3b), reproduced from Ref. [33], shows a comparison between experimental and theoretical cross-sections for the  $^{89}$ Y(n, $\gamma$ ) reaction. The dashed curve is calculated by using the real interaction (3), while the continuous line represents the results of calculations with the complex interaction (6). The strengths  $v_1$  and  $w_1$  are adjusted to obtain similar cross section magnitudes, the other parameters being unchanged. Agreement similar to that shown in Fig. 3b) was also obtained for neutron radiative capture by  $^{208}$  Pb and  $^{140}$ Ce [32-34].

The disturbing point with formula (6) is that the weight of the imag-

inary term is determined by an effective strength  $\tilde{w}_1 = 4b \frac{4 < r >}{< r^2 >} w_1$ . This masked the fact that the effective strength of the imaginary term used in [32-34] was much greater than the strength of the real term  $(\tilde{w}_1^2 \gtrsim 10v_1^2)$  and, therefore, the real term could often be neglected, as shown in Ref. [35].

For this reason we prefer to derive the imaginary part of the interaction in the same way as was done in Ref. [22] for the real part, and to use a complex nucleon-nucleus coupling interaction with a volume form for both the real and the imaginary parts, and furthermore with the same normalization, that is



- Fig.3. a) Cross section for  $(n,\gamma)$  transitions to all single-particle levels of <sup>20</sup> Pb. The continuous and dashed curves are calculated [24] with the same set of parameters by using the volume form (4) of the interaction in the former case and the surface form (3) in the latter.
  - b) Cross section for  $(n,\gamma)$  transitions to single-particle levels below 4.5 MeV in 90 Y. The continuous and dashed curves are calculated [33] by using the complex interaction (6) and the real interaction (3) respectively. The strengths v<sub>1</sub> and w<sub>1</sub> are adjusted to obtain similar cross section magnitudes, the other parameters being unchanged.

(7)

$$h(r) = (v_1 + i w_1)\xi(r)$$
.

The relative weights of the real and imaginary parts of this interaction are given directly by the values of  $v_1$  and  $w_1$ , which are obviously quite independent of each other. Cross sections for capture by  $^{89}$ Y,  $^{140}$  Ce and  $^{208}$ Pb have been calculated [35-36] using formula (7) with  $v_1 = w_1 = 130$  MeV giving a satisfactory agreement between theory and experiment (see section 4). With the strengths used, both parts of the interaction are obviously needed to obtain a magnitude agreement between theory and experiment: the neglecting of either one of the two terms would give cross section values of about half the calculated ones.

# 3. EXISTING COMPUTER CODES

Computer codes for direct-semidirect calculations are available at least at Oxford [4], Bologna [5], Studsvik [7], Ljubjana [8], Grenoble [17], Tokyo [19], New York [20], Obninsk [21], Budapest [31] and Livermore [37] as results, for example, from papers quoted. To our knowledge only the CNEN Bologna computer code descriptions have been published [38-39].

The CNEN Bologna DIRCO-programme calculates the direct and semidirect dipole-capture cross sections for individual single-particle bound states at a given incident neutron energy. The total cross section is then given as the sum of the contributions over all possible final states. Paper [38] contains the mathematical formulation, a detailed description of the programme written in FORTRAN IV language for an IBM 360/75 computer, the input list and the output data of a calculation for a test run.

The programme has great flexibility as to the optical potential which can be used for the continuum state. The continuum partial wave functions are supplied by a subroutine programme which solves the Schrödinger equation by the method described in detail in Ref. [40]. A subroutine programme calculates the radial part of bound-state wave functions solving the Schrödinger equation by an iterative procedure, as described in Ref. [41]. The radial integrals ought to be calculated over all space in order to include the internal (r<R) contribution as well as the external (r>R) one. In the programme integration is carried out until the integral values become constant (the difference between the minimum and maximum values of two near integrals is lower than 0.1%).For prudence's sake, neutron capture integrals are calculated up to r=30 fm with an integration step of 0.04 fm.

The programme outputs are the cross sections and the radial integrals (real part, imaginary part and square) for individual transitions at a given neutron energy. If so desired, the integrals and wave functions can be print ed as functions of the nuclear radius. The wave functions can also be plotted versus the nuclear radius. The plots of the cross sections (total, direct, semidirect and interference) and of the radial integral squares versus the incident neutron energy can be given, too.

Fig. 4. reproduced from Ref. [11], shows an example output of the DIRCO-programme referring to the 208Pb(n, $\gamma$ ) reaction at 10 MeV neutron energy. The radial dependence of the 3d 5/2 bound-state wave function and of the real and imaginary parts of the f 7/2 continuum wave functions are given in Fig. 4a). The coupling function (3) used for calculating the semidirect integrals is plotted in the inset. The real and imaginary parts of the semi-direct radial integral for the f 7/2  $\Rightarrow$  d 5/2 transition is shown in Fig. 4b).

The CNEN Bologna SPEC-programme calculates the  $\gamma$ -ray spectra from  $(n,\gamma)$  reactions according to direct and semidirect mechanisms. Report [39] contains a description of the method used in calculating the spectra, a detailed description of the programme written in FORTRAN IV language for an IBM 360/75 computer, the input list and the output data of a calculation given as an example.

The programme assumes the DIRCO-code [38] as a means of calculating the cross sections which are then spread over an energy interval corresponding to the resolution of the spectrometer, in order to get the calculated spectra. In the programme, either a Gaussian spread or the response function of the spectrometer can be inserted. Thus, the SPEC-programme output is more useful for analyzing the results of a given experiment than for predicting theoretical  $\gamma$ -ray spectra which can be directly obtained from the DIRCO outputs.



- Fig.4. a) The radial dependence of the 3d<sub>5/2</sub> neutron bound-state wave function in <sup>209</sup>Pb (\_\_\_\_\_\_). The real (\_\_\_\_\_\_) \_\_\_\_\_) and imaginary (\_\_\_\_\_\_) parts of the f<sub>7/2</sub> continuum wave function.
  - b) The real (- -) and imaginary (- - -)parts of the semidirect radial integral for the  $f_{7/2} \rightarrow d_{5/2}$  transition of the  $^{208}$ Pb $(n,\gamma)$  reaction at 10 MeV neutron energy. The function (3) used for calculating this integral is plotted in the inset.

# 4. COMPARISON BETWEEN THEORY AND EXPERIMENT

Here only recent calculations [35-36] carried out by using form (7) of the particle-vibration coupling will be referred to. A rapid survey of previous comparisons between theory and experiment has been given in sub--section 2.2.

It seems advisable to limit the comparison between theory and experiment to prompt y-ray spectra following the radiative capture of fast neutrons, as well as to cross sections deduced from integration of these  $\gamma$ -ray spectra. The radiative capture cross sections obtained by means of the im-proved activation technique [30,42-44] can also be useful for comparison, disregarding earlier activation data, when not confirmed by more recent In fact, until recently, the data measurements. on fast neutron radiative capture measured by means of these two techniques were contradictory and a comparison with the theoretical estimates was conse quently very dubious. The 14 MeV  $(n,\gamma)$  cross sections, deduced from integra tion of recorded  $\gamma$ -ray spectra, generally increase with the mass number up to about A % 60, then showing a very smooth mass dependence, with values around 1 mb. The activation cross section values differed markedly from the above results, especially for deformed nuclei, for which values higher by more than a factor of 10 were often obtained. After the Kantele and Valkonen [42], and successive [30,43-44], measurements it seems established beyond all doubt that a large number of the previous activation results were overestimated, through a failure to make the necessary corrections for secon dary neutrons produced in the sample, in target heads and in surrounding materials. The data at the isolated energy of 14 her connections and the validity of ered very significant for the sake of comparison. Therefore, the validity of [25,26] only on three medium and heavy nuclei, <sup>89</sup>Y, the theory is tested in [35-36] only on three medium and heavy nuclei,  $^{89}\mathrm{Y}$ ,  $^{140}\mathrm{Ce}$ ,  $^{208}\mathrm{Pb}$ . For these nuclei the partial (n,  $\gamma$ ) cross sections for capture to various single-particle states have been measured at neutron energies covering a large part of the giant-dipole resonance by using the method of integrating the corresponding gamma-ray spectra.

Calculations are carried out with renewed versions of the DIRCO and SPEC codes, using complex interaction (7) with a volume form for both real and imaginary terms and as strengths  $v_1 = w_1 = 130$  MeV. The incident and bound-state wave functions are calculated by using the optical potential [45] and its real part respectively. The depth of the bound state potential is adjusted to give the experimentally known binding energy of the single-particle states. The cross sections are calculated with the values for the energy and width of the giant dipole state obtained from measured photoneutron reactions. The information on the neutron level structure (single particle states, binding energies and spectroscopic factors) is deduced from (d,p) reaction experiments.

Fig. 5 shows a comparison between the calculated [36] cross section for  $(n,\gamma)$  transitions to low energy levels in <sup>141</sup>Ce and the experimental points [33] and [16]. In this case the agreement is excellent, while for capture by <sup>80</sup>Y and <sup>208</sup>Pb some disagreement still persists at lower neutron energies.

A second kind of experimental data which can be useful for comparison with theory are the measured  $\gamma$ -ray spectra. As is known, the intensity of high-energy gamma rays calculated on the basis of statistical theory decreases smoothly with energy. The experimental  $\gamma$ -ray spectra following capture of 6-15 MeV neutrons by  $^{89}$ Y,  $^{140}$ Ce and  $^{208}$ Pb [18,33] clearly reveal an excess of high-energy gamma rays and several peaks that may correspond to neutron capture to single-particle orbitals as predicted by the direct-semidirect theory. In order to compare theoretical and experimental  $\gamma$ -ray spectra the cross sections for individual single-particle bound states are corrected for detector  $\gamma$ -ray efficiency and then spread over the energy interval corre-



Fig.5. Cross section for  $(n,\gamma)$  transitions to levels below 3.5 MeV in <sup>141</sup>Ce. The experimental points are taken from Ref.[33] (dots) and Ref.[16] (square). The curve is calculated [36] by using complex interaction (7).



Fig.6. Comparison between experimental [18] and calculated [36] spectra of high-energy photons emitted in the  $^{208}Pb(n,\gamma)$  reaction.

sponding to the response function of the spectrometer.

In Fig. 6 the calculated [36] and observed [18]  $\gamma$ -ray spectra follow ing the capture of 9.2 MeV and 13.2 MeV neutrons by <sup>208</sup>Pb are shown. Here the measured data, given in relative intensity, are plotted versus the excitation energy of the final nucleus. The individual single particle states used in calculations are indicated at the top of the figure. As can be seen, the essential features of the spectral shapes are reproduced. In this case, as in the others, a discrepancy between measured and calculated spectra generally remains for high excitation energies up to the neutron separation energy  $B_{_{\rm N}}$ .

#### 5. POSSIBLE THEORETICAL DEVELOPMENTS

Comparisons between experimental points and direct-semidirect calculations with a complex form of the particle-vibration coupling have shown that: 1) a discrepancy between measured and calculated spectra is observed for high excitation energies in the residual nucleus (see Fig. 6); 2) in some cases the discrepancy on the left-hand side of the giant resonance peak is not fully removed.

A way of increasing the calculated cross sections on the low energy side of the giant resonance may be sought by including the quadrupole capture contribution. For neutron capture the direct quadrupole cross section is obviously negligible owing to the low effective charge [46]. The situation is different with semi-direct capture. In this case preliminary calculations [47-48] show that quadrupole capture, though less important than El capture, should not be neglected. Inclusion of quadrupole capture, however, cannot help one to reproduce observed  $\gamma$ -ray spectra at high excitation energies.

A possible contribution to the cross section by the compound nucleus mechanism, as indicated in earlier papers (see, for example [5,7-8], still seems the best way for removing the two above mentioned discrepancies. In fact, such a contribution should be greater, as required, for the lower neutron energies considered. On the other hand, the intensity of high-energy gamma-rays in the statistical spectrum decreases smoothly with energy and this will help to reproduce observed spectra better. Therefore a superposition of three mechanisms (compound nucleus, direct and semidirect capture) seems to be a way for improving explanations as to experimental data.

The direct-semidirect theory has been extended to deformed nuclei [17]. The results obtained confirm that the calculated cross sections are similar, using either a spherical or a deformed potential. The use of that more complicated formulation for application purposes is probably a little premature until such time as greater accuracy in experiment and better reliability in calculations have been obtained. The same can be said for extension of the model to non-zero-spin target nuclei.

At present, however, further refinement of the model seems not to be the most urgent task. Indeed, 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  $v_1$  and  $w_1$ . 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.

# 6. APPLICATIONS OF THE MODEL

As a first and straightforward application, the direct-semidirect model can be used to calculate  $(n,\gamma)$  cross sections. For this purpose it is sufficient to employ the DIRCO-code to obtain curves like those shown in Figs. 3 and 5.

The direct-semidirect model also allows us to calculate: a) the gamma-ray spectra following radiative capture of fast monochromatic neutrons, b) the effective cross sections for the production of photons with energies greater than 8-10 MeV. In what follows, interest will centre on these two applications of the theory.

It is well known that radiative capture is only one of the possible reactions for producing photons in the MeV region, the dominant reactions being  $(n,n'\gamma)$ ,  $(n,X\gamma)$  and fission reactions in the heaviest nuclei. But the dominant mechanism for producing several MeV gamma-rays is probably radiative capture. Thus the cross sections for the production of photons with energies greater than  $\sim 10$  MeV should be calculated by using the direct-semidirect model.

Following the model, the incident neutrons are captured to states in the final nucleus which have a single-particle structure. This implies that to a given neutron energy there should correspond a group of monochromatic emitted gamma-rays. The predictions of theory are shown in <u>Fig. 7</u> for the same gamma-ray spectra considered in <u>Fig. 6</u>. Obviously the spectra plotted in <u>Fig. 7</u> are calculated without introducing corrections relating to the detec tor gamma-ray efficiency or spectrometer response function, as was necessary for comparison with the results of the particular experiments considered. For this purpose the output of the DIRCO programme is directly used.

As can be seen from Fig. 7, the relative importance of capture to a given level varies with neutron energy and reaches its maximum for gamma-rays corresponding to the giant resonance energy (13.42 MeV for  $^{208}$ Pb). The neutron binding energy in  $^{209}$ Pb being 3.94 MeV, this means that low excitation energy levels are favoured at 9.2 MeV neutron energy and vice versa at 13.2 MeV.

Of course, the case of strictly monochromatic neutrons is not the most important in technology. Attention should also be devoted to those neutrons having a continuous spectrum of energies, for example resulting from scattering and other nuclear reactions after passing through the first wall, the blanket and other structures of a fusion reactor.

As an example, the 8-20 MeV gamma-ray effective production cross section for the  $^{208}$  Pb(n, $\gamma$ ) reaction is plotted in <u>Fig. 8</u>. The three curves are calculated for a unitary initial neutron flux with three different incident energy distributions ranging from 4 to 15 MeV. The neutron energy distributions, shown in the inset to <u>Fig. 8</u>, are: a) a uniform incident energy distribution; b) a distribution, reproduced from Ref. [49], correspond ing to part of the neutron leakage spectrum for a 25-cm diameter niobium sphere with a source of fission neutrons at the centre; c) a distribution, also reproduced from Ref. [49], corresponding to part of the neutron leakage spectrum for a 76-cm diam. iron sphere with a D-T source at the centre.

The radiative capture cross section for the  $^{208}Pb(n,\gamma)$  reaction has been calculated for more than a hundred neutron energies ranging from 4 to 15 MeV. The photons produced in a given photon-energy interval have been summed together after their weighting to the relative incident neutron flux, thus obtaining the photoproduction yields corresponding to the different neutron distributions considered. As can be seen from the figure, the curve obtained for a uniform neutron energy distribution (dots) reproduces the distinctive feature of the giant dipole resonance, while the curves corresponding to a fission (dot-dashed line) or a fusion (continuous line) neutron



Fig.7. Calculated gamma-ray spectra for radiative capture of monochromatic neutrons by <sup>208</sup>Pb.

source are displaced towards lower or higher energies and exhibit different peaks, their trends being influenced both by the neutron distribution and the level structure of the target nucleus.

Similar calculations have been performed for the  $^{93}$ Nb(n, $\gamma$ ) reaction, [35], which is of greater interest in fusion reactor technology. For this nucleus, however, the information on the level scheme and spectroscopic factors is rather poor. Therefore the final states have been chosen equal to those predicted by the shell model for spherical nuclei and the bound-state wave functions and energies have been calculated as in Ref. [15]. As for <sup>208</sup>Pb the real and imaginary strengths of the isospin part of the optical potential have been taken equal to 130 MeV.

The photoproduction cross sections for the  $^{93}$ Nb(n, $\gamma$ ) reaction, corresponding to the same three incident neutron distributions considered for  $^{208}$ Pb are plotted in <u>Fig. 9</u>, reproduced from Ref. [35]. The difference in the level structure of these two nuclei gives rise to some differences in the trends of calculated curves. Obviously, calculations like those for the  $^{93}$ Nb(n,  $\gamma$ ) reaction are not so reliable as for  $^{208}$ Pb. In fact, calculations for lead were checked on experimental (n, $\gamma$ ) data covering the whole region of the dipole giant resonance and available for capture to different single particle states, whereas the calculations for  $^{93}$ Nb were compared only with



the measured [15] isolated value at 14 MeV.

Fig.8. Calculated cross sections for the production of 8-20 MeV photons from neutron radiative capture by <sup>208</sup>Pb. The 4-15 MeV neutron incident energy distributions considered are shown in the inset. The dotted curve is obtained for a uniform neutron energy distribution; the dot-dashed and continuous lines for neutron spectra from fission and fusion sources respectively.



Fig.9. The same as in Fig. 8 for capture by  $9^{3}$ Nb.

### 7. CONCLUDING COMMENTS

The cross sections for production of high energy (>8 MeV) photons, which are difficult to obtain experimentally, can be estimated by using direct-semidirect model calculations. To our knowledge no accurate experimental data are available for a direct comparison with calculated curves like those plotted in <u>Figs. 8-9</u>. An indirect comparison of calculated photoproduc tion cross sections can be made against experimental data, such as those considered in section 4. In spite of the encouraging results achieved in indirect comparisons, further experimental data are needed in order to adequate ly predict unknown data. In fact, calculations account for the magnitude of the (n,  $\gamma$ ) cross sections and their dependence on the incident energy as well as for the shape of observed  $\gamma$ -ray spectra, but the reliability of the estimated data is closely related to the calculation parameters - till now very uncertain. This refers to bound, continuum and giant-dipole state parameters and especially to the crucial parameters  $v_1$ , and  $w_1$ . It seems however that, when some experimental points are available in the 6-14 MeV neutron energy range, the curves calculated by adjusting the  $v_1$  and  $w_1$  strengths to these points can give a reasonable estimate of the cross section behaviour in the energy region considered.

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### STATISTICAL CHARACTERISTICS OF EXCITED NUCLEI

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#### ABSTRACT

The author reviews the principal methods of giving a theoretical description of the statistical characteristics of excited nuclei. It is shown that in many cases such characteristics can be analysed successfully on the basis of the thermodynamic relations of the non-interacting quasiparticle model in which the shell structure of the spectrum of singleparticle states is taken into account. Specific peculiarities of the appearance of correlation effects of the superconducting type in the level density of nuclei are discussed. The collective branch of coherent oscillations of excited (heated) nuclei is investigated in the randomphase approximation. The contribution of vibrational and rotational movements to the level density is estimated. Combinatorial methods of calculating level density are considered and their correspondence to the thermodynamic description is discussed.

#### INTRODUCTION

Nowadays a statistical approach is frequently adopted for describing many phenomena associated with the formation and decay of a compound nucleus. Such an approach is appropriate when one is analysing processes of the observed characteristics to which many states of the excited nucleus make an averaged contribution. As a result of averaging, individual peculiarities of states become more or less negligible and only the most general properties of the group of states under investigation need be included among the statistical characteristics. Study of extensive spectroscopic material on the structure of low-lying levels has shown that most phenomena in excited nuclei are attributable to different manifestations of two aspects of nucleon motion: singleparticle motion of nucleons in a self-consistent field and coherent collective movements of the self-consistent field (or of a large group of nucleons)[1].

In the analysis of average cross-sections for various nuclear reactions, attention is usually focused on the single-particle motion of nucleons. The success of the Fermi-gas model in describing excitation functions, evaporation spectra, etc. has shown that the statistical characteristics of excited nuclei are very similar to the characteristics of a degenerate ideal Fermi-gas[2]. In a nucleus, however, such a gas possesses a number of specific peculiarities due, on one hand, to the presence of pronounced shell structures in the spectrum of the singleparticle states and, on the other, to the influence of pair correlations on the motion of excited particles. The most characteristic examples of the experimental manifestation of these effects and the methods for describing them theoretically will be considered in the first two sections of this paper.

A great deal of attention is paid to the collective aspect of nucleon motion in the study of the structure of low-lying nuclear levels; however, the role of such motion in a highly excited nucleus is only just beginning to be studied. In this area, the main difficulties are connected with the lack of proper experimental information about the behaviour of the statistical characteristics of nuclei over a wide range of excitation energies. When discussing the influence of collective effects on the thermodynamic properties of nuclei, we are therefore obliged at present to rely mainly on the results of the theoretical calculations described in the third section.
In the fourth section we present combinatorial methods of calculating the level density of excited nuclei, discuss the main results of such calculations and consider their agreement with the results of the thermodynamic description.

#### 1. SHELL EFFECTS IN THE LEVEL DENSITY OF NUCLEI

In a statistical description, the probability of different processes is proportional to the phase-space volume occupied by a system with given integrals of motion. In a nucleus, this volume is determined by the density of the excited states (or levels). Simple analytical relations for the density of the states  $-\omega(U) - of$  a nucleus with a given excitation energy U and the density of the levels  $-\varrho(U,J) - of$ a nucleus with a given angular momentum J are obtained in the Fermi-gas model[3]:

$$\omega(U) = \frac{\sqrt{\pi'}}{12 \, a^{\sqrt{4}} \, U^{5/4}} \exp\left\{2\sqrt{a} \, U\right\}$$
(1a)

$$\rho(U, J) = \frac{2J+1}{24\sqrt{2}\sigma^3} \omega(U) \exp\left\{-\frac{(J+1/2)^2}{2\sigma^2}\right\} (1b)$$

Here  $\sigma^2$  is the spin dependence parameter and  $a = \pi^2 g/\sigma$  is the level density parameter, which is proportional to the density of single-particle states g near the Fermi energy. In the Fermi-gas model, the equations of state determining the dependence of the excitation energy U, the entropy S and other thermodynamic functions of the nucleus on its temperature t also have a simple form:

# $U = at^2$ , S = 2at, $\sigma^2 = m_f^2 g^{t}$ (2)

Here  $m_f^2$  is the average value of the square of the projection of the angular momentum of single-particle states lying close to the Fermi energy, which can also be associated with the moment of inertia of a nucleus  $F_o = gm_f^2$ . The interrelationship of the thermodynamic functions (2) with the density of the states of an excited nucleus (1) is obvious.

In the quasiclassical approximation it is easy to estimate the parameters of the Fermi-gas model:

$$a = 2\left(\frac{\pi}{3}\right)^{4/3} \frac{mr_0^2}{\hbar^2} A$$
,  $f_0 = \frac{2}{5}mr_0^2 A^{5/3}$  (3)

where m is the nucleon mass,  $r_0$  the radial parameter and A the mass number.

The directest and most reliable information about the level density of excited nuclei is derived from experimental data on the density of neutron resonances. Considerable work[4] is being done at present on the analysis of these data on the basis of the relations (1)-(3), and the results demonstrate convincingly two characteristic features of excited nuclei: (a) a significant difference between the level densities of nuclei having the same excitation energy but differing with regard to the parity of the number of protons or neutrons; (b) pronounced shell effects in the dependence of the level density of nuclei on mass number. Generally, in order to allow for differences in the level densities of even and odd nuclei, in the relations of the Fermi-gas model one uses the effective excitation energy defined as

$$U^{*} = U - \begin{cases} \delta_{Z} + \delta_{N} & \text{for even-even nuclei} \\ \delta_{Z} & \delta_{N} & \text{for nuclei with even Z or N} \\ 0 & \text{for odd-odd nuclei} \end{cases}$$
(4)

where b is an analogous correction for even-odd differences in the nuclear masses. The value obtained through such an analysis for the ratio of the level density parameter a to the mass number is shown in Fig. 1[5]. Experimental values of the shell correction to the mass formula are shown in the lower part of this figure. The marked decreases of the ratio a/A in the region of magic nuclei and the clear correlation between this ratio and the value of the shell correction point to the importance of shell effects in the behaviour of the statistical characteristics of excited nuclei.

The correlation between the level density parameter a and the shell correction to the mass formula or the degree of degeneracy of the subshells closest to the Fermi energy is often used in constructing semiempirical dependences of the parameter a on nuclear composition [4-6]. With this approach it is possible to obtain fairly simple and convenient systematics of the behaviour of the level density of nuclei at excitation energies close to the neutron binding energy. However, one must be cautious when using the results of such systematics for a wide range of excitation energies. Since the parameter a does not depend on the excitation energy with such a description, the shell effects in the level density of a nucleus will remain unchanged at any higher excitation energies. Obviously, this result contradicts the basic physical ideas about the influence of shell effects on the properties of excited nuclei.

To obtain a more correct description of the statistical characteristics of a nucleus it is necessary, when calculating the thermodynamic functions (2), to take into account the discrete character of the spectrum of the single-particle states of nuclei[7]. In that case, the relations for entropy S, energy U, number of particles N and Z, etc. will have the form

$$S = \sum_{v} \left\{ p \varepsilon_{v} \overline{n}_{v} + ln \left(1 + e^{-\beta \varepsilon_{v}}\right) \right\}$$

$$U = \sum_{v} \varepsilon_{v} \left\{ \overline{n}_{v} - \Theta(\varepsilon_{v}) \right\}, \quad N = \sum_{v} \overline{n}_{v} \quad (5)$$

$$\sigma^{2} = \sum_{v} m_{v}^{2} \overline{n}_{v} (1 - \overline{n}_{v})$$

where  $\varepsilon_{v}$  is the energy of single-particle states computed from the corresponding chemical potential (proton or neutron),  $\overline{n}_{v} = [1 + \exp \beta \varepsilon_{v}]^{-1}$  represents the average occupation numbers of these states at a temperature  $t = 1/\beta$  and the sum over v embraces all single-particle states with allowance for their degeneracy. For a given scheme of single-particle states, the relations (5) enable one to calculate the thermodynamic functions and the density of the states of an excited nucleus without introducing any additional parameters. To demonstrate the influence of shell effects more clearly and to trace the difference between the behaviour of the thermodynamic functions (5) and the Fermi-gas dependence (2), it is useful to determine quantities equivalent to the parameter a and to  $F_0$  (or  $m_f^2$ ) of the Fermi-gas model:

$$a' = S^{2}/4U , \quad \bar{a} = \frac{\pi^{2}}{6}\beta \sum_{v} \bar{n}_{v} (1 - \bar{n}_{v}) , \quad ^{(6)}$$
$$\overline{m^{2}} = \frac{\pi^{2}}{6a}\beta \sum_{v} m_{v}^{2} \bar{n}_{v} (1 - \bar{n}_{v}) , \quad \mathcal{F}_{II} = \beta \sigma^{2} .$$

The results of the calculation of these quantities for a single-particle scheme of Nilsson potential levels are shown in Fig. 2[8]. At a low excitation energy, U = 7 MeV, the "shell decreases" well known from the study of the behaviour of experimental values of the parameter a (Fig. 1), show up clearly in the behaviour of a' and  $\bar{a}$ . Similar effects occur for moment of inertia  $F_{||}$  and the parameter  $m^2$ . At fairly high excitation energies ( $\geq 100$  MeV), the shell non-uniformities of the single-particle spectrum no longer exert an appreciable influence on the thermodynamic characteristics of the nucleus, and the mass number dependence of the quantities (6) has a fairly simple form:

$$\bar{a} = 0.105 \text{ A } \text{MeV}^{-1},$$

$$\overline{m^2} = 0.290 \text{ A}^{2/3} (1 - \frac{2}{3} \text{ c}),$$

$$\overline{f_1} = 1.85 \cdot 10^{-2} \text{ A}^{5/3} (1 - \frac{2}{3} \text{ c}) + \frac{\pi^2}{\text{MeV}}.$$
(7a)

where **E** is the parameter of quadrupole deformation of the Nilsson potential. For the Saxon-Woods potential level scheme, the results of numerical calculations of the analogous parameters differ somewhat in the value of the corresponding coefficients:

$$\overline{a} = 0.090 \text{ A MeV}^{-1}, \qquad (7b)$$

$$\overline{m^{2}} = 0.263 \text{ A}^{2/3} (1 - \frac{2}{3} \text{ C}), \qquad (7b)$$

$$\overline{f_{11}} = 1.44 \cdot 10^{-2} \text{ A}^{5/3} (1 - \frac{2}{3} \text{ C}) \text{ T}^{2}/\text{MeV}.$$

The difference between the coefficients in the relations (7a) and (7b) is due to the finite depth and the diffuseness of the Saxon-Woods potential. On the whole, the coefficient values obtained through numerical calculations are fairly close to the values obtained in the quasiclassical approximation - see expressions (3). A discrepancy in the estimated values of  $\overline{m^2}$  is due to the spin-orbit component of single-particle potentials.

\*/ Translator's note - My quotation marks, indicating a literal translation.

The dependence - considered above - of the thermodynamic functions of the nucleus on the shell structure of the single-particle spectrum and the close link between this dependence and the size of the shell correction to the mass formula have been discussed in detail in many works[11, 12]. Moreover, a considerable amount of experimental data demonstrating such a dependence in the behaviour of the level density of nuclei has accumulated[13, 14]. Apparently, the clearest manifestation of shell effects is observed in the energy dependence of cross-sections for the fission of "cis-actinide"\*/ nuclei by alpha particles[14]. The excitation energy dependence - derived from these data - of the level density parameter of the neutron  $(a_n)$  and fission  $(a_r)$ channels for a <sup>210</sup>Po nucleus is shown in Fig. 3[15]. The behaviour of the parameter  $a_n$  in the near-magic <sup>209</sup>Po nucleus is in good agreement with the shell dependence of the parameter a considered above. The characteristics of the fission channel relate to strongly deformed transitional configurations of the nucleus, for which the shell nonuniformities of the single-particle spectrum are far less pronounced than for near-magic nuclei and hence the behaviour of the parameter a, at high energies hardly differs from that of a Fermi-gas (the reason for the break at low energies will be considered in the next section).

Despite the success in describing the energy dependence of the thermodynamic characteristics of the nucleus, in many cases the results of theoretical calculations do not reproduce the absolute value of the observed neutron resonance density (or the absolute value of the derived level density parameter). Although these discrepancies are not large, they are of a systematic nature; hence, when analysing different experimental cross-sections, one cannot at present confine oneself to the results of purely theoretical level density calculations - it is necessary to link them in absolute terms to the available experimental data.

The phenomenological description of the level density parameter at different excitation energies, which is of practical use, can be obtained if one takes as one's starting point the effects considered above: strong correlation of  $a_{exp} (B_n^*)$  with the shell correction in the mass formula (Fig. 1)

<sup>\*/</sup> Translator's note - My quotation marks, indicating a translation based on the analogy with "transactinide".

and disappearance of shell effects in the behaviour of a(N,Z) at high excitation energies (Fig. 2). In this case, the energy dependence of the level density parameter may be presented in the form

## $a(v, N, z) = \tilde{a} \{1 + f(v) \ SW(N, z) / U \}$ (7)

where  $\tilde{a}$  is the asymptotic value of the parameter a at high excitation energy ( $\tilde{a} = \alpha A + \beta A^{2/3}$ ) and f(U) = 1 - exp (- $\gamma$ U) is a dimensionless function determining the energy behaviour of the level density parameter. The structure of the relations for a(U), f(U) and  $\tilde{a}$  is obtained by theoretical reasoning, while the values of the parameters (in MeV<sup>-1</sup>)

$$\alpha = 0.114, \quad \beta = 0.162, \quad \gamma = 0.054$$
 (8)

were found by analysing the experimental values of the level density parameter  $a_{exp}$  ( $B_n^*$ )[16]. The fundamental difference between such phenomenological systematics of the behaviour of the parameter a(U,N,Z)and the similar systematics considered in Refs 4 and 6 lies in correct allowance for changes in the influence of shell effects as a function of nuclear excitation energy.

It should be noted that the resulting description of the Fermi-gas level density parameter (7) will be more correct at excitation energies exceeding the neutron binding energy since the effects of residual interactions in this systematics are taken into account only by the empirical choice of a correction for the even-odd differences (4). At lower energies ( $\leq 6-7$  MeV), an important role is played in nuclei by pair correlations, which do not reduce to a simple excitation energy shift, and the dependence a(U) has a more complex form than that predicted by the relation (7). Even in this energy region, however, the influence of pair correlations on nuclear level density can be simulated within the framework of Fermi-gas relations by a corresponding energy dependence of the parameter a (see  $a_f$  for E > 10 MeV in Fig. 3). The role of pair correlations will be considered more fully in the next section. The parameter value found with the phenomenological description  $(\alpha = 0.114 \text{ MeV}^{-1})$  appreciably exceeds the quasiclassical estimate  $(\alpha = 0.075 \text{ MeV}^{-1} \text{ for } r_0 = 1.2 \text{ fm})$ . This difference points to the existence of fairly strong factors which are not taken into account by the non-interacting quasiparticle model and which increase the level density of excited nuclei in the neutron resonance region by a factor of 20-100. The most natural explanation for this increase lies in the collective effects which play a decisive role in the formation of the spectrum of low-lying nuclear levels. We shall later revert to this question.

#### 2. INFLUENCE OF PAIR CORRELATIONS ON LEVEL DENSITY

The influence of residual interactions of the correlation type on the properties of the ground and low-lying levels of atomic nuclei has been the subject of fairly extensive study[17, 18]. Such an interaction has much in common with the correlation interaction of electrons in a superconductor, so that the mathematical apparatus of superconductivity theory has been used successfully for describing correlation effects in nuclei[19]. The use of this apparatus in level density calculations has been considered in many works (7, 10-12; see also the references given in these works).

The application of superconductivity theory to the analysis of the statistical properties of excited nuclei is associated with a number of peculiarities attributable to the microcanonical character of the problem in question. For the sake of simplicity, in discussing these peculiarities we shall confine ourselves to a one-component system of N particles. In this case, the density of the states can be presented in the form

$$\omega(\mathbf{U}) = \frac{1}{2\pi\sqrt{D}} \exp(\mathbf{S}) \qquad (9)$$

where the main thermodynamic functions of the system are determined by the relations [20]

$$S = 2 \sum_{k} \{\beta E_{k} \overline{n}_{k} + ln (4 + e^{-\beta E_{k}})\}, \qquad (10)$$

$$U = \sum_{k} \{\sqrt{\epsilon_{k}^{2} + \Delta_{o}^{2}} - E_{k} (4 - 2\overline{n}_{k})\} + \frac{\Delta_{o}^{2} - \Delta^{2}}{G}, \qquad (10)$$

$$D = 4 \{ [\sum_{k} E_{k}^{2} \overline{n}_{k} (4 - \overline{n}_{k})] [\sum_{k} \overline{n}_{k} (4 - \overline{n}_{k})] - [\sum_{k} \epsilon_{k}^{2} \overline{n}_{k} (4 - \overline{n}_{k})]^{2} \}$$

Here  $\bar{n}_k = [1 + \exp \beta E_k]^{-1}$  is the average number of quasiparticles in the k-th state,  $E_k = [\epsilon_k^2 + \Delta^2]^{1/2}$  is their energy, G is the correlation interaction constant of the particles and  $\Delta$  is the system correlation function, which is determined by the equation

$$\frac{2}{G} = \sum_{k} \frac{1 - 2\bar{n}_{k}}{E_{k}}$$
(11)

At zero temperature, the relations (10) and (11) determine the energy  $U_{\triangle}$  and the correlation function  $\triangle_{\triangle}$  of the ground state of the system.

The correlation function decreases with rising temperature and becomes zero at temperature  $t_c$ ; this temperature corresponds to phase transition from the superconducting to the normal state. At this point the thermodynamic functions (9) have a break characteristic of phase transitions of the second kind. Above the critical temperature, the relations (10) coincide with the relations (5) of the non-interacting particle model.

It should be noted that in many works the relations for the preexponential factor D differ from the above relation - see expressions (10). The temperature dependence of such D [11] have a discontinuity instead of a break (a similar discontinuity also appears in the density of the states) at the phase transition point. The occurrence of such a discontinuity is due to a number of inaccuracies tolerated when applying a variation transformation of superconductivity theory to the level density problem. If the variation transformations are carried out more rigorously, no discontinuity occurs in the temperature dependence of the pre-exponential factor or the level density itself[20].

The influence of pair correlations on the behaviour of the thermodynamic characteristics of the nucleus is shown in Fig. 4 for the continuous spectrum approximation  $(2\sum_{k} \rightarrow g\delta d\epsilon$ , where g is the density of single-particle states). The critical temperature  $t_c$  is connected with the correlation function of the ground state  $\triangle_c$  by the relation

 $t_{c} = 0.567 \Delta_{0},$  (12a)

and corresponds to the excitation energy

$$U_{c} = \frac{\pi^{2}}{6}gt_{c}^{2} + \frac{1}{4}g\Delta_{o}^{2}$$
(12b)

The quantity  $g\Delta_0^2/4$  determines the energy which must be expended in order to destroy the pair correlations in a cold system (for t = 0); it is usually called the condensation energy. Above the phase transition point, the temperature dependence of the entropy, moment of inertia, etc. coincides with the analogous dependence of these functions in the Fermi-gas model; their energy dependences in this region will also coincide if the effective excitation energy

$$U^* = U - \frac{1}{4} g \Delta_0^2 \tag{13}$$

is used in the superfluid model of the nucleus. It should be noted that, with the transition from temperature to energy dependence, the difference between the behaviour of  $\omega(U)$  and  $\sigma^2(U)$  in the non-interacting particle model and the superfluid model will not be very pronounced; consequently, for experimental observations of such differences it is necessary to have data for a fairly wide range of excitation energies. For a narrow range of energies the differences can be reduced slightly through an appropriate choice of parameters. The presence of shell non-uniformities in the single-particle spectrum leads to a dependence of the level density parameter a and of  $m^2$  on nuclear excitation energy. Allowance for such a dependence does not change the basic pattern of the behaviour - considered above - of the thermodynamic functions of the superfluid model, but it does lead to non-linear deformations of the scales on the axes in Fig. 4. For a given single-particle spectrum, the density of the states of an excited nucleus can be calculated with the help of the relations (9)-(11), which are easily generalized for the case of a two-component (protons and neutrons) system[7, 11].

The most characteristic feature of the superfluid model is, of course, the phase transition from the superconducting to the normal state. This transition has been the subject of thorough experimental investigations in the case of superconductors, and the behaviour of the thermodynamic functions corresponding to it is in very good agreement with the results of the theoretical description[19]. As the atomic nucleus is an isolated system, the nature of the phase transitions occurring in it is more complex. In order to understand it, one should perhaps consider in greater detail the structure of the states excited in the nucleus. In the non-interacting quasiparticle model, the excited states can be characterized by - among other integrals of motion - the number of excited quasiparticles n. The methods for solving such a problem and the corresponding calculations of  $\omega_n(U)$  are considered in Ref. 21.

The density of all the states of a nucleus can be obtained by summing the n-quasiparticle densities over all energetically possible configurations:

$$\omega(U) = \sum_{n} \omega_{n}(U) \qquad (14)$$

It should be noted that, for a system with an even number of particles, the numbers of quasiparticles in the sum over n assume only even values  $(n = 0, 2, 4 \dots)$ , whereas  $n = 1, 3, 5 \dots$  etc. for odd values of N. The density of the states  $\omega_n$  determines the statistical weight of the different n-quasiparticle configurations, and with its help one can obtain any average characteristic of the system under consideration:

$$A(\upsilon) = \sum_{n} A_{n}(\upsilon) \omega_{n}(\upsilon) / \sum_{n} \omega_{n}(\upsilon) \quad (15)$$

For the sake of simplicity, we shall again confine ourselves to a one-component system of particles[22]. The energy dependence of the density of the states  $\omega_n$ , the spin dependence parameter  $\sigma_n^2$  and the correlation function  $\Delta_n$  for a system with an even and an odd total number of particles N is shown in <u>Fig. 5</u>. The same figure shows the results of calculations of the total density of the states (14) and of the mean values of  $\sigma^2$  and  $\Delta(U)$  calculated with the help of the relation (15) and also the behaviour of analogous values obtained by means of the traditional thermodynamic description (10) and (11). For a system with a fixed number of quasiparticles, the correlation function of configurations with  $n < g\Delta_0/3$  is non-zero throughout the excitation energy range - i.e. such systems are always in a superconducting state. Systems with  $n \ge g\Lambda_0/3$  can be in both the superconducting and the normal phase, but the normal-phase region is at lower excitations than the superconducting one - i.e. the phase transition has an energetically inverse direction relative to the phase transition of the traditional description. For states with any n, with increasing excitation energy the correlation functions  $\Lambda_n(U)$  grow and tend towards  $\Lambda_0$  for  $U \rightarrow \infty$ . If one calculates the density of the states  $\omega(U)$  and the average statistical characteristics of the system on the basis of the relations (14) and (15), then - strictly speaking - at U<sub>c</sub> no breaks occur in the energy dependence of the density of the states and the spin dependence parameter. With growing excitation energy the mean correlation function decreases, but it does not vanish at U<sub>c</sub>.

With the traditional thermodynamic description of the characteristics of an excited nucleus, the appearance of phase transition is the price we pay for the simplifications employed in solving the problem. These simplifications are associated with the fact that the Hartree-Fock-Bogolyubov variation transformation is performed in the simplest statistical variant - i.e. its coefficients are derived from the condition that the most probable system configuration is best described by a non-interacting quasiparticle Hamiltonian. In this case, the phase transition merely reflects the fact that, above U, the correlation function is zero for the most probable n-quasiparticle configuration. In superconductors described by a canonical ensemble, the number of excited quasiparticles is very high, the average characteristics of the system virtually coincide with the most probable ones and the temperature dependence of the correlation function  $\Delta(t)$  is observed directly in experiments. For a nucleus, which is an isolated system and described by a microcanonical ensemble, configurations differing from the most probable one make a substantial contribution to the density of the nuclear states, and this manifests itself in the fact that the most probable value of the correlation function differs from the averaged value.

The refinements relate mainly to the question of the fundamental difference between the thermodynamics of a nucleus and the thermodynamics of the systems in a thermostat. However, if a phase transition in a nucleus is not understood in too rigorous a sense (as the actual existence of two well separated phase states) and one speaks of two regions with different energy dependences of the statistical characteristics of the nucleus, then the above thermodynamic approach, (9)-(11), may be regarded as a fairly good approximation for calculating the density of the states of excited nuclei.

The results of the calculations of the density of states (14) for a system with an even and an odd number of nucleons, presented in Fig. 5, also enable one to understand the reason for the occurrence of even-odd differences in the behaviour of the statistical characteristics of nuclei. It can be seen that, with the selected origin from which the excitation energy is reckoned (zero excitation energy corresponds to a quasiparticle vacuum), even-odd differences in the total density of the states exist only in the region of low excitation energies when one- or twoquasiparticle configurations are essentially possible. The density of the states of both even and odd nuclei averaged over these structures is described fairly well by the results of the thermodynamic calculations (9)-(11). However, a quasiparticle vacuum is the ground state only for a system with an even number of particles; for an odd system, the ground state corresponds to the energy of the lowest single-particle excitation. With the usual determination of the excitation energies, the energy scale for an odd system must therefore be shifted by an amount equal to the difference in energy between the lowest level and a quasiparticle vacuum. In the continuous spectrum approximation, this difference

$$U_{4} = \Delta_{0} \left(1 - \frac{1}{2g\Delta_{0}}\right) \tag{16}$$

and it is possible to show that in the general case it is the difference between the condensation energies calculated for the ground state of a system with an odd number of particles without and with allowance for blocking by an unpaired particle of the single-particle level nearest the Fermi energy. Thus, even-odd differences in level density are determined solely by a shift of the origin from which the excitation energy is reckoned, and the thermodynamic description of the density of the states (9)-(11) with a corresponding shift of the origin of (16) is applicable to both even and odd nuclei.

It is not difficult to extend the results obtained to the description of a two-component system. In that case, one must take into account the

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influence of unpaired particles on the condensation energy of the proton and neutron components. As the single-particle spectrum of nuclei has a very non-uniform shell structure, the condensation energy will be strongly dependent on the number of nucleons. The results of condensation energy calculations for different single-particle level schemes are presented in Ref. 22. Despite the significant differences as regards the condensation energy itself, the energy difference as between an even and an odd system is about 1 MeV, which is on the whole in accordance with the extent of the phenomenological shift  $\delta$  of the effective excitation energy of the Fermi-gas model (4). For nuclei with A ~ 60, the experimental data on the level density over a wide range of excitation energies enable one to verify directly the validity of the model considered. The results of the level density calculations are shown in Fig. 6 together with the corresponding experimental data. The theoretical curves are based on the relations (9)-(11) for a single-particle Saxon-Woods potential level scheme; they describe fairly well the nuclear level density differences with different nucleon number parities.

When the Fermi-gas model relations (1) are used for analysing the energy dependence of the density of the states, the presence of two regions with different energy dependences of the thermodynamic functions of the nucleus (phase transition in the sense considered above) should manifest itself in a change in the energy dependence of the Fermi-gas level density parameter a. This effect is observed directly in the behaviour of the fission channel level density shown in Fig. 3. The results of a similar analysis, covering a larger number of nuclei, of cross-sections for the fission of "cis-actinide" nuclei are presented in Ref. 23. The systematically observed break in the energy dependence of the Fermi-gas parameter of the fission channel level density enables one to obtain a fairly reliable estimate of the critical energy U and to derive the value of the correlation function for transitional states of a fissioning nucleus,  $\Delta_{f} \simeq 0.9$  MeV. This value of  $\Delta_{f}$  is close to the analogous nuclear ground state parameter  $\Delta_{0} = 12.5 \text{ A}^{-\frac{1}{2}} \text{ MeV}$ , which points to fairly weak dependence of the correlation function on deformation of the nucleus. Phase transition is now observed with a high degree of assurance also in the energy dependence of the effective moments of inertia determining the angular distribution of induced fission products [15, 24]; the value of  $\Delta_{f}$  derived from these data accords well with the results of the analysis of the energy dependence of the parameter  $a_{f}^{\bullet}$ . Summing up the results of the analysis of the experimental data one can say that the superfluid model gives a natural explanation of the main peculiarities of the energy dependence of the density of the states of excited nuclei. Taking into account the shell structure of the singleparticle spectrum by means of this model, for near-magic nuclei it is also possible to obtain a description of the absolute value of the observed level density; at the same time, one cannot obtain such a description for deformed nuclei[25, 26]. Thus, the question - raised at the end of the preceding section - of the contribution of collective motion to the level density of excited nuclei remains even after interactions of the correlation type have been taken into account.

#### 3. CONTRIBUTION OF COLLECTIVE MOTION TO THE LEVEL DENSITY

A great deal of attention is paid to collective phenomena in nuclei when spectroscopic information about the characteristics of low-lying levels is being analysed. It has proved possible, within the framework of the generalized model of the nucleus, to understand and systematize the extensive experimental material relating to the collective properties of nuclei[1]. In considering the interconnection of collective excitations with the single-particle or uncorrelated multiparticle motion of nucleons in nuclear theory, considerable use is made of the mathematical methods of quantum field theory, by means of which a quantitative description of the structure of most low-lying nuclear states is obtained[18, 27, 28]. In this connection there naturally arises the question of the influence of collective effects on the level density and other statistical characteristics of highly excited nuclei. In its general form such a problem is very complex, and methods sufficiently rigorous to solve it have not yet been devised. It is reasonable to expect, however, that a fully satisfactory approximate solution will be found through appropriate generalization of the models employed for describing low-lying collective levels.

The level density calculation methods considered above are based on the idea of the energy of a nucleus as the sum of all kinds of combinations of the energy of excited non-interacting quasiparticles. Attention was long ago[2] drawn to the considerable difference between such an approach and the phenomenological methods of constructing a spectrum of low-lying levels in the generalized model of the nucleus, where the collective motion of the nucleus separates adiabatically from the single-particle motion (see also Ref. 29). If such an adiabatic separation of collective and single-particle degrees of freedom is used in constructing any of the highly excited states of the nucleus, then the total density of the excited states can be presented in the form

### $\omega(U) = \omega_{in}(U) k_{vibr} k_{rot}$ (17)

where  $k_{rot}$  and  $k_{vibr}$  are the coefficients of the level density increase due to the rotational and vibrational modes and  $\omega_{in}$  corresponds to the previously considered density of the states of the non-interacting quasiparticle model. By means of the saddle point method, which is well known in statistical physics, one can show that  $k_{rot}$  and  $k_{vibr}$  are for practical purposes equivalent to the contribution of the rotational and hence the vibrational modes to the statistical sum of the system. In the adiabatic approximation, the calculations of such a contribution are analogous to the calculations of the statistical sum of a two-atom ideal gas:

$$k_{rot} = \sum_{j=0,2...} (2j+1)e^{-j(j+1)/2j} \simeq \mathcal{F}_{1}t$$
 (18)

$$k_{vim} = \prod (1 - e^{-\omega_i/t})^{-2\lambda_i - 4}$$
(19)

Here  $F_{\perp}$  is the moment of inertia of the nucleus relative to the perpendicular to the symmetry axis of the direction and  $\lambda_i$  is the multipolarity of a vibrational mode with energy  $\omega_i$ . The relationship between temperature t and nuclear excitation energy U in the adiabatic approximation is determined by the equations of state of the non-interacting quasiparticle model. In the calculation of  $k_{rot}$  it was assumed that the shape of the excited nucleus was axially symmetric; otherwise  $F_{\perp}t$  should be doubled. It can readily be seen that adiabatic allowance for rotational motion increases the density of the states and the level density of an excited deformed nucleus by a factor of 50-100 compared with the results of calculations

based on the non-interacting quasiparticle model. The increase in the level density due to vibrational motion will be appreciable if there are low-energy modes with  $\omega_i \leq 1-2$  MeV in the excited nucleus. The liquid drop estimate of the energy of the lowest quadrupole oscillations,  $\omega = 100 \ \text{A}^{-5/6}$  MeV, implies an increase in the level density of intermediate and heavy nuclei by a factor of 2-8 at excitation energies close to the neutron binding energy.

When the level density increase due to collective motion of the nucleus (17) is taken into account, there is a considerable improvement in the theoretical description of the experimental data on the density of the neutron resonances [26, 30]. When collective motion is separated out in this adiabatic fashion, however, there remains completely untouched a whole series of very important questions about differences of collective phenomena in a nucleus at different excitation energies, about the mixing of collective with single-particle motion, etc. To resolve these questions it is necessary to develop more rigorous methods for considering collective motion against a background of multiparticle motion which are equivalent to the microscopic methods of describing the low-lying collective levels of nuclei [18, 27, 28]. With these methods, various modifications of perturbation theory are used for constructing the spectrum of the elementary single-particle or collective excitations of a system of interacting particles in the ground state. As a matter of fact, in the case of the statistical description of an excited nucleus we encounter a similar problem: it is necessary to determine the spectrum of the elementary excitations of a system characterized by temperature - i.e. a system which is with equal a priori probability in any of the energetically attainable states. Methods for solving this problem have been considered by Ignatyuk 31, who has shown that, in the random phase approximation, the Bose branch of the spectrum of the elementary single-phonon excitations of a heated nucleus is determined by the secular equation

$$4=2 \varkappa \sum_{k,k'} |f_{kk'}|^2 \left\{ u_{kk'}^2 (i-\bar{n}_{k'}-\bar{n}_{k'}) \frac{E_{k'}+E_{k'}}{(E_{k'}+E_{k'})^2 - \omega^2} \right\}^{(20)}$$
  
- $V_{kk'}^2 (\bar{n}_{k'}-\bar{n}_{k'}) \frac{E_{k'}-E_{k'}}{(E_{k'}-E_{k'})^2 - \omega^2}$ 

where  $f_{kk}$ , represents matrix elements and  $\times$  is the constant of the corresponding effective multipole-multipole residual interaction;  $u_{kk} = u_k v_k + v_k u_k$  and  $v_{kk} = u_k u_k - v_k v_k$  ( $u_k$  and  $v_k$  being coefficients of the variation transformation in the superfluid model of the nucleus). The contribution of such excitations to the thermodynamic characteristics of the system are described by the relations

$$\Delta S = \pm \sum_{i} (2\lambda_{i}+1) \left\{ \frac{\beta\omega_{i}}{2} \operatorname{cth} \frac{\beta\omega_{i}}{2} - \ln(2\operatorname{sh} \frac{\beta\omega_{i}}{2}) \right\},$$
  

$$\Delta U = \pm \sum_{i} (2\lambda_{i}+1) \frac{\omega_{i}}{2} (\operatorname{cth} \frac{\beta\omega_{i}}{2} - 1), \qquad (21)$$
  

$$\Delta D = \pm \sum_{i} (2\lambda_{i}+1) \frac{\omega_{i}^{2}}{4} (\operatorname{sh} \frac{\beta\omega_{i}}{2})^{-2}.$$

where the superscript corresponds to the roots of the secular equation (20) and the subscript to its poles. The poles of this equation determine the excitation energy of a pair of non-interacting quasiparticles, whereas the roots determine the energy of coherent excitations in a system of interacting quasiparticles.

The contribution of the Bose branch of the elementary excitations to the density of the states can be presented approximately in the form

$$k_{vibr} = e^{\Delta m_s} = \prod k_{vibr}(\omega_i) / k_{vibr}(\omega_i^{\circ}) \qquad (22)$$

where  $k_{vibr}(\omega_i)$  is the adiabatic contribution of a vibrational mode with given frequency  $\omega_i$  and multipolarity  $\lambda_i$  to the statistical sum of the system. In expression (22),  $\omega_i$  relates to the roots of the secular equation and  $\omega_i^{o'}$  to its poles. If there is a small difference between  $\omega_i$  and  $\omega_i^{o'}$ , the ratio of the statistical sum components corresponding to them tends towards unity, so that the main contribution to  $k_{vibr}$  will be made just by the strongly collectivized frequencies. The appearance of the statistical sum of the poles in the relation (22) and of analogous sums in the relations for the thermodynamic functions of the system reflects the non-adiabatic nature of the collective effects considered.

The results of calculations of  $k_{vibr}$  for the <sup>58</sup>Fe nucleus are shown in Fig. 7 by way of example. The continuous curve represents the results of amplification coefficient calculations obtained for the total spectrum of the roots and poles of the secular equation  $(20) - i_{\bullet}e_{\bullet}$  with allowance for the nuclear temperature dependence of the position of the roots of the secular equation. The dashed curve represents the amplification coefficient calculated for the phonon and pole spectrum of a cold nucleus. With rising temperature the coherence of the quadrupole low-frequency excitations decreases; this manifests itself in a weakening of their influence on the level density of the excited nucleus. The inverse relationship, corresponding to a strengthening of the coherent effect, applies in the case of octupole phonons. It should be noted that the value of the coefficient k<sub>vibr</sub> obtained in calculations with the spectrum of the roots and poles of a cold nucleus is determined almost completely by the energy of the first single-phonon excitation, whereas a fairly large number of secular equation roots contributes to  $k_{vibr}$  in a heated nucleus. For  $t \neq 0$ , the spectrum of such roots is very dense and contains many low-frequency roots with  $\omega_{i}$  <t (especially in deformed nuclei). As a rule, not one of these roots is strongly collectivized, but taken together they can make an appreciable contribution to entropy and to the level density increase coefficient.

The appearance of low-frequency coherent modes with  $\omega_i \ll t$  in the spectrum of solutions to the secular equation (20) is to some extent due to the inaccuracy of the random phase approximation, within the framework of which the damping of elementary excitations of the nucleus is not taken into account.

The problem of the microscopic description of damping is fairly complex and a satisfactory solution has not yet been found in nuclear theory, even for zero temperatures. However, an approximate estimate of the influence of the effects due to damping can be obtained with the help of the relations characterizing the lifetime of elementary excitations in Fermi-liquid theory[32]. The analogue of the coherent excitations of a nucleus in Fermi-liquid theory is zero-point sound, the region of existence of which is determined by the inequality  $\omega > \tau^{-1}$ , where  $\tau$  is the reaction time or the mean lifetime of the quasiparticles. It is to be expected that, in a nucleus, with allowance for damping the spectrum of solutions to the secular equation (20) will be limited by a similar inequality and only solutions satisfying this inequality will fit into calculations of the thermodynamic characteristics of an excited nucleus. On the basis of experimental data relating to the imaginary part of the optical potential it is possible to obtain an estimate of the relaxation time  $\tau^{-1} = (1.5) \times 10^{-2} t^2$  MeV. For such a value of  $\tau$ , the limitations on the spectrum of solutions to the secular equation will be unimportant for most spherical nuclei at temperatures below 1.1.5 MeV; in the case of deformed nuclei, however, when one is calculating level density increase coefficients they must be taken into account throughout the temperature range.

It should be emphasized that the coherent excitations determined by the secular equation (20) do not correspond to real fluctuations of the shape of a nucleus in some highly excited state. They should be interpreted only in a statistical sense as the collective component of the density matrix in an excited nucleus. Such coherent modes should manifest themselves in experiments as resonance peaks in the strength functions of radiation transitions or in other, analogous statistical characteristics of nuclei. These questions have been considered in greater detail elsewhere[33].

The results of calculations of  $k = k_{rot} k_{vibr}$ , the coefficients of the level density increase due to the combined influence of the vibrational and rotational motion of heated nuclei, are presented in Fig. 8 for excitation emergies equal to the neutron binding energy (for spherical nuclei  $k = k_{vibr}$ ). By taking this increase into account one is able to obtain, over a wide range of mass numbers, a fairly good theoretical description of the available experimental data on the mean distance D<sub>exp</sub> between the neutron resonances (see lower part of Fig. 8)[34].

The adiabatic separating-out of rotational poles appears to be reasonably justified at excitation energies which are not very high. With rising energy there should be a breakdown of such coherent motion equivalent to the breakdown of the vibrational excitations of heated nuclei. At present, however, we have no convincing estimates of the temperature or excitation energy range where such a breakdown occurs. Thus, despite the satisfactory description of the experimental data, the description of the rotation of a heated nucleus entails many

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unresolved questions the study of which requires the development of more rigorous microscopic methods for separating out rotational motion which are equivalent to the methods employed in the case of cold nuclei[35].

#### 4. COMBINATORIAL CALCULATIONS OF LEVEL DENSITY

In recent years, a successful description of experimental data on the density of neutron resonances has been obtained on the basis of combinatorial methods of calculating the energies of the highly excited multiparticle states of nuclei[36, 37]. The same effective Hamiltonian is used in such calculations as in the thermodynamic methods - considered above - for describing the statistical characteristics of nuclei; however, the relations employed in level density calculations differ appreciably with the two approaches and this is reflected to some extent in the results.

To demonstrate these differences, we show in Fig. 9 the results of calculations of the energy dependence of the density of the states of a spherical nucleus, <sup>58</sup>Fe, and a deformed nucleus, <sup>238</sup>U, performed using the non-interacting particle model. For the sake of simplicity, the effect of blocking was not taken into account in the combinatorial calculations - i.e. the correlation function of the excited nucleus coincided with the correlation function of the ground state. The results in Fig. 9 of the thermodynamic calculations of the density of the states allow one to trace the influence of this approximation. The most characteristic feature of combinatorial calculations is the nonmonotonic energy dependence of the level density, which is particularly pronounced in spherical nuclei. However, the value for the density of the states averaged over such fluctuations is virtually the same for the two approaches, and the results of the thermodynamic calculations of level density agree fairly well with those of the combinatorial calculations even at low excitation energies.

The divergences between the results of the calculations of different authors are due mainly to differences in single-particle level schemes or to other, additional approximations employed in coherent variants of the calculations. A quantitative calculation of such divergences requires more detailed discussion and lies outside the scope of this work.

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In the analysis of experimental data on the level density of excited nuclei, equiprobable distribution of states of positive and negative parity is usually assumed. Combinatorial calculations of level density have shown that, at excitation energies below the neutron binding energy, for a number of nuclei the contribution of states of different parity can differ appreciably from the equiprobable contribution[36, 37]. This result is not a specific feature of combinatorial calculations; it may be obtained with a simpler, statistical approach. For this purpose we shall use an estimate - obtained in Ref. 2 - of the parity distribution of the states of a system of non-interacting quasiparticles. If an excited quasiparticle is with probability  $p_{-}$  in a state with negative parity and with probability  $p_{+} = 1-p_{-}$  in a state with positive parity,  $P_{+}$  is determined by the relations

$$P = \frac{1}{2} \{1 - m | 1 - 2p_{-} |^{n} \}, P_{+} = 1 - P_{-}$$
(23)

where  $m = \begin{cases} 1 \text{ for even-even and odd-odd nuclei,} \\ 1 \text{ if } p_{-} < \frac{1}{2} \\ -1 \text{ if } p_{-} > \frac{1}{2} \end{cases} \text{ for odd nuclei}$ 

These relations hold for any values of n (not necessarily those enumerated), so that they can be used to describe the parity distribution of the states of an excited nucleus, n being taken to be the mean number of excited quasiparticles. Since the single-particle levels in the shell model are characterized by a certain parity, the thermodynamic relations necessary for calculating n and p\_will have the form[38]

$$n = \sum_{v} g_{v} \bar{n}_{v} , p_{\pm} = \sum_{v} p_{v}^{(\pm)} g_{v} \bar{n}_{v} / n ,$$

$$p_{v}^{(+)} = \frac{1}{2} \left[ 4 - (-1)^{\ell_{v}} \right] , p_{v}^{(+)} = 4 - p_{v}^{(-)}$$
(24)

Here  $\bar{n}_v$  is the mean population of single-particle levels with given orbital momentum  $\ell_v$  and degree of degeneracy  $g_v$ .

The results of calculations of the excitation energy dependence of n, p\_ and P\_ are shown in Fig. 10 for the most typical nuclei. The Saxon-Woods potential level scheme was used in the calculations and the influence of pair correlations on the thermodynamic characteristics of the nucleus was taken into account on the basis of the relations (10) and (11). It should be noted that allowance for pair correlations has only a slight influence on the results of the calculations, since the peculiarities of the behaviour of n and p are determined mainly by the single-particle level scheme. Values of P have been obtained for  $^{58}$ Fe and <sup>124</sup>Te nuclei which are very close to the results of combinatorial calculations[37] - indicated by dots in Fig. 10. In Fig. 11 we present the results of calculations of n and p for a one-component system of quasiparticles. The continuous curves show the behaviour of the proton component and the dashed curves that of the neutron component. The calculations were performed for a temperature t = 0.7 MeV, which corresponds on average to excitation energies close to the neutron binding energy. These results enable one to trace the dependence of the effects considered on nucleon composition. Although for a onecomponent system p departs quite considerably from  $\frac{1}{2}$ , for nuclei close to the beta-stability valley the influence of the proton and neutron components cancels out in many cases and the density distribution of the excited states is close to the equiprobable distribution.

At low excitation energies, information about the parity distribution of the states of a nucleus can be obtained from the spectroscopic characteristics of low-lying levels. This information is in good qualitative agreement with the results of the calculations considered above, but the number of such levels is usually too small for discussion of the statistical pattern in their distribution. Information about the influence of parity on the density of the states of highly excited nuclei can be derived from data on the density of the neutron resonances formed by s- and p-neutrons and from data on the ratio of the mean radiation widths of such resonances. In this connection, considerable interest has been aroused by the publication in recent years of experimental data on p-resonance parameters[39]; analysis of these data may refine our ideas about the statistical characteristics of highly excited nuclei. Summarizing the above discussion, it would seem reasonable to say that we understand different aspects of the appearance of shell effects in highly excited nuclei and have a coherent description of the correlation effects in such nuclei; the available experimental data confirm the validity of the theoretical models employed.

At the same time, there are in highly excited nuclei many phenomena whose interpretation involves the collective motion of nucleons. The theoretical description of these phenomena is still far from satisfactory. We have considered here only the simplest and most typical examples of such a description. The available experimental data qualitatively confirm many results of the theory, but the absence of data for a wide energy range greatly hampers the quantitative comparison of results. For a critical verification of the theoretical models we need a marked qualitative improvement and an expansion of the experimental information about the processes occurring through the compound nucleus stage; in many cases we also need more rigorous analysis of the accumulated experimental data.

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#### FIGURE CAPTIONS

- Fig. 1. Mass number dependence of the Fermi-gas parameter of level density a (top) and the shell correction to the mass formula (bottom).
- Fig. 2. Results of calculations of the parameters a', ā, m<sup>2</sup> and F<sub>||</sub> in the non-interacting particle model for excitation energies of 7 MeV (a) and 100 MeV (b): • - calculations with a spherical single-particle potential; o - calculations with a deformed potential.
- Fig. 3. Energy dependence of the level density parameter of the fission  $(a_f)$  and neutron  $(a_n)$  channels derived from an analysis of cross-sections for the reaction  ${}^{206}Pb(\alpha,f)[15]$ . In the low-energy region, the value of parameter a obtained for adjacent nuclei from an analysis of neutron resonances is shown.
- Fig. 4. Temperature dependence of the thermodynamic characteristics of the superfluid model of the nucleus (continuous curves) and the Fermi-gas model (dot-and-dash curves).
- Fig. 5. Energy dependence of the n-quasiparticle and average characteristics of a system ( $g = 18.3 \text{ MeV}^{-1}$ ,  $\Delta_0 = 0.85 \text{ MeV}$ ). The figures by the curves denote the number of quasiparticles. The continuous curves are for a system with an even number of quasiparticles and the broken curves are for one with an odd number; the dot-and-dash curves correspond to the thermodynamic description (10).
- Fig. 6. Energy dependence of the level density of even-even, odd and odd-odd nuclei.
- Fig. 7. Temperature dependence of the level density increase coefficients of the <sup>58</sup>Fe nucleus due to quadrupole 2<sup>+</sup> and octupole 3<sup>-</sup> vibrational modes (continuous curves). The broken curves show the values of similar coefficients obtained for the vibrational-mode spectrum of a cold nucleus. The excitation energy corresponding to the temperature in question is indicated along the upper scale.

- Fig. 8. The coefficient of the level density increase due to collective effects (top) and the description of the mean distance between neutron resonances obtained when it is taken into account (bottom).
- Fig. 9. Comparison of combinatorial (histogram) and thermodynamic level density calculations. The thermodynamic calculations of  $\omega$  (U) were performed for a correlation function  $\Delta = \Delta_0$  (continuous curve) and with allowance for the temperature dependence  $\Delta(t)$  (broken curve).
- Fig. 10. Excitation energy dependence of the mean number of excited quasiparticles n, the probability p\_ and the relative contribution of P\_ states of negative parity to the nuclear level density. The black dots indicate the results of Ref. 37 for  $58_{\rm Fe}$  and  $124_{\rm Te}$ .
- Fig. 11. Nucleon composition dependence of the values of n and  $p_{-}$  for a one-component system. The continuous curves indicate the behaviour of the proton component and the broken ones that of the neutron component. The calculations were performed for spherical nuclei "heated" to a temperature t = 0.7 MeV.





Fig. 2

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Fig. 3









Fig. 7



Fig. 8








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Fig. 11

# THE OPTICAL MODEL WITH PARTICULAR CONSIDERATION OF THE COUPLED-CHANNEL OPTICAL MODEL

by

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ABSTRACT

A review concerning the role and efficiency of the optical model with an emphasis on the coupled-channel model in neutron nuclear data evaluation is presented. After a short survey of the theoretical and numerical frame of these models, recent practical uses and limitations are discussed. Improvements and parameterisation procedures are suggested.

#### 1. INTRODUCTION.

At the present time theoretical models, including the optical models, are being used increasingly (i) to complete evaluated data files for nuclei for which few measured data are available, or (ii) to provide in the near future reasonable neutron cross-sections for nuclei for which no data are available or even measurable. These data files generally include, for a given nucleus, many different crosssections within a large energy range (0-20 MeV). In this context, what is really required concerning theoretical evaluation tools, such as the optical model, is a treatment as physical and systematic as possible that will allow extrapolations with reasonable confidence. Recently a "Critique of nuclear models and their validity in the evaluation of nuclear data" has been discussed, including optical model problems, at the EANDC Meeting at Tokyo [1]. A typical example of nuclei for which many nuclear data are required and theoretical calculations planned, is the transactinium nuclides which were the subject of the last IAEA Advisory Group Meeting on Transactinium Isotope Nuclear Data at Karlsruhe in November 1975. The theoretical aspects of the evaluation of the data for these nuclei have been reviewed by LYNN [2].

Many years ago [3], it was well established that the use of an optical potential, that is a complex single-particle field, is necessary to account for the gross-structure of the energy-averaged neutron elastic (and total) cross-sections as a function of the incident energy or mass-number. This structure consists of broad (few MeV width) resonances [4] which cannot be taken into account by the old black nucleus model [5]. Today, the theoretical foundation of the optical model from a many-body point of view is well understood since pioneering works such as those by BROWN [6] and FESHBACH [7]. Recent books and reviews describe extensively these aspects [8-11]. A discussion of the "microscopic" developments of the optical potential is largely beyond the scope of this paper, because it appears, as discussed in the following, that the nuclear data evaluators are unfortunately not yet ready to take advantage of such sophisticated tools. Rather, we shall focus our attention on some recent aspects of the evaluation problems in the framework of the currently used phenomenological optical models, and especially of the coupled-channel ones. Recent lectures about the role and efficiency of nuclear models, including optical models, in nuclear data evaluation have been given by BENZI [12].

Therefore the main emphasis in this paper will be :

(i) to briefly review the theoretical and numerical frame in which the phenomenological optical model calculations are currently carried out for evaluation purposes,

(ii) to survey some recent practical uses and limitations of this model, and

(iii) to suggest ways to improve, in the near future, the use and especially the parameterisation procedure of the model in order to contribute, with other models, to more reliable and more accurate theoretical extrapolations.

This explains the following organization we adopt.

#### 2. THE COUPLED CHANNEL OPTICAL MODEL

2.1. Introduction

A few years ago, one asked the (spherical) optical model (0.M) to re produce qualitative and quantitative features of elastic scattering of nucleons. While it was successful, physicists went further and hoped the optical model would give a qualitative and quantitative description of elastic scattering and inelastic scattering from collective states. The model was then extended in connection with the development of spectroscopic studies for low-lying collective excited states of nuclei. This extention of 0.M. to inelastic scattering of particles from collective excited states led to the coupled-channel optical model (C.C.O.M.).

Typically, scattering data were chosen as tests of nuclear models, and the coupled-channel optical model was (and remains) a tool of spectroscopic studies. T. TAMURA has published a review article on the formalism and applications to spectroscopy [13] .

For the evaluation of neutron scattering data, the point of view about the C.C.O.M. is different : essentially, the main work does not consist in testing the validity and accuracy of phenomenological collective models, but in an estimation of required quantities such as elastic, inelastic and total cross sections. It is supposed that collective wave functions of the target and the O.M, in their actual C.C. formulation, are good enough. Then, most of the work, for a nucleus, lies in finding a parameterisation of the potential wich gives good agreement with most of experimental data over a wide energy range. At the same time, when the parameters obtained are supposed to be realistic enough, one can deduce, from O.M. calculations, transmission coefficients wich are included , for example, in statistical model calculations (cf. papers at this Meeting about statistical model).

#### 2.2. Theoretical frame of the C.C.O.M.

Before going in practical aspects and assumptions of the usual formalism, it is instructive to come back to the fundamentals of this model [14, 15]. Antisymmetrisation effects and transfer reactions (pick-up, stripping,...) will be neglected.

Let us assume that we have available model wave functions  $\phi_{\alpha I}$  for the states of the target nucleus A. They are eigenfunctions of the model Hamiltonian H<sub>A</sub> :

$$(H_A - E_{\alpha I}) \phi_{\alpha I} (A) = 0$$
 (1)

I is a quantum number for the spin states of target,  $\alpha$  a set of complementary quantum numbers for the complete description of target states.

The total Hamiltonian for the interacting system is written as :

$$H = H_A + T + V$$
(2)

with :

T = kinetic energy of relative motion ; V = interaction potential.

It is important to note that V must be consistent with  $H_A$ : if  $\phi_{\alpha I}(A)$  are phenomenological collective states (vibrational or rotational), V must reflect this choice through deformation parameters. If  $\phi_{\alpha I}(A)$  are microscopic wave functions, V must be the sum of two-body potentials.

The wave function  $\Psi$  , which describes the scattering process, must be a solution of :

$$(H - E) \Psi = 0 \tag{3}$$

with : E = total energy of the system in C.M.

Now, one has to determine  $\Psi$  using spectroscopy tools, remembering that total angular momentum J and parity  $\pi$  of the interacting system are good quantum numbers. The expansion for  $\Psi$  can be expressed in the usual notation as :

$$\Psi = \frac{1}{r} \sum_{J\pi M} \sum_{c} U_{c}(r) \phi_{c}(x,A)$$
(4)

where :

- r is the radial coordinate of the relative motion ;

- x is a set of variables on which the interaction depends ;

 c is the usual notation for the set of quantum numbers that denotes a reaction channel;

$$-\phi_{c}^{J\pi M}$$
 includes target and projectile wave functions, exclu-  
ding the r-dependent components.

The radial wave functions  $u_c^{J\pi}$  are solutions of the following equations :

$$\left[\widetilde{\mathbf{T}}_{\mathbf{c}} - \mathbf{E}_{\mathbf{c}} + \langle \phi_{\mathbf{c}}^{\mathbf{J}\pi\mathbf{M}} | \mathbf{V} | \phi_{\mathbf{c}}^{\mathbf{J}\pi\mathbf{M}} \rangle \right] \mathbf{u}_{\mathbf{c}}^{\mathbf{J}\pi} = -\Sigma_{\mathbf{c}\neq\mathbf{c}}, \langle \phi_{\mathbf{c}}^{\mathbf{J}\pi\mathbf{M}} | \mathbf{V} | \phi_{\mathbf{c}}^{\mathbf{J}\pi\mathbf{M}} \rangle \mathbf{u}_{\mathbf{c}}^{\mathbf{J}\pi}, \quad (5)$$

In the matrix elements of V, the integration is done over all variables but the radial coordinate ; in (5), we have the usual notations for  $\widetilde{T}_{c}$  :

 $\widetilde{T}_{c} = \frac{\hbar^{2}}{2m} \left[ -\frac{d^{2}}{dr^{2}} + \frac{\ell_{c}(\ell_{c} + 1)}{r^{2}} \right] \qquad (m \text{ is the reduced mass}),$ 

and :

 $E_c = E - E_{\alpha I}$  .

The equation (5) is an infinite coupled channel (c,c') system. Within experimental conditions, it is possible to obtain, generally, informations(angular distribution, polarisation) only for a small number of collective levels (low-lying ones). Thus, it is desirable to reduce the infinite system (5) to a finite one, while saving transition amplitudes for these few excited states. This is obtained when one changes the potential V into an effective, complex, non-local and energy dependent potential U [14]. Its imaginary part, Im U, is interpreted as a simulation of all the reaction processes which are not explicitly considered : non low-lying excited states, transfer reactions, antisymmetrisation effects and compound processes.

#### 2.3. Usual formulations of the C.C.O.M.

When one wishes to solve coupled-channel equations with effective potentials (optical potentials), some further approximations are needed.

2.3.1. The usual effective potential

It is not issued from a separate study, though its derivation from fundamental concepts is in progress [16].

The real part, Re U, reflects the matter density of the target nucleus ; in a first approximation, its central part is assumed to have a SAXON-WOODS shape and a strength whose energy variation has a simple form. This point will be discussed later. In Re U is included a spin-orbit potential whose exact expression was given by BLAIR and SHERIF and RAYNAL [17]; this term is mainly connected with the interpretation of polarization phenomena. The determination of the shape of the imaginary part, Im U, is more difficult. At low energy, the incoming nucleon can't occupy a state in the Fermi sea (Pauli principle), so the absorption, occuring at the surface of the target nucleus, is sharp in shape there ; very often, one chooses for it a derivative of a SAXON-WOODS form. When a wide energy range is explored, volume absorption must be added in competition with the surface absorption. This is apparent in many experimental data analyses, and is supported by microscopic calculations of Im U [16]. The energy dependence of Im U, and Re U, will be discussed later.

## 2.3.2. Folding model for the effective potential

In order (i) to decrease the number of free parameters and (ii) to understand the physical behaviour of the different terms of a phenomenological optical potential, it is desirable to adopt potential shapes suggested by the microscopic derivations of the optical model. In this context, many aspects of the so-called folding model have been extensively surveyed by SINHA [11]; this review includes many references. Let us only recall here that the real part of the entrance channel optical potential may be conveniently represented by folding in a two-body interaction v with the target nucleonic density distribution  $\rho(r)$ . Neglecting exchange effects arising from the antisymmetrisation of the wave functions of the incident nucleon with those of the target nucleons, this folding term takes the simple form :

$$\operatorname{ReU}(\mathbf{r}) = \int \rho(\mathbf{r}') \, \mathbf{v}(|\mathbf{r}'-\mathbf{r}|) \, \mathrm{d}^3\mathbf{r}' \,. \tag{6}$$

Despite of the crude approximations employed (identical shapes for neutron and proton density distributions, SAXON-WOODS form-factor for  $\rho(r),...$ ), GREENLEES et al. [18] have demonstrated that this folding form, using a complete realistic <u>free</u> two-body interaction v was able (i) to reduce the number of independent parameters in an optical model analysis, and (ii) to reproduce reasonably well the proton elastic scattering data at high energy.

Actually, the expression (6) including such a free interaction v, together with a realistic  $\rho(r)$ , represents the first-order microscopic optical potential in a perturbation series with respect to V.

Furthermore, one can account approximately for the second-order realpart contributions by including in (6) a bound-state <u>effective</u> twobody interaction. Several studies have been hopefully undertaken using various forms of v [11]. Let us just mention the recent so-called D1 soft-core effective interaction which is density dependent and with finite range. This interaction, successfully applied in predicting properties of finite nuclei by the Hartree-Fock-Bogoliubov (H.F.B.) methods [19], has not yet been tested in the continuum region. Such H.F.B. calculations are also able to provide realistic  $\rho(r)$  functions.

Nevertheless, it is worth while to emphasize the importance of the exchange terms which, in particular, are believed to contain most of the energy dependence of the optical model. These terms are calculated with the mixed density  $\rho(\mathbf{r',r})$  and the exchange components of the two-body interaction  $\mathbf{v}$ . Thus, taking into account the nonlocality resulting from such effects, the Schrödinger equation, in coordinate-configuration, leads to the difficult problem of solving integro-differential (possibly coupled) equations. In this context, the use of a matrix method will be discussed later on (cf. Ch. 3.2) for spherical potentials.

The imaginary optical potential arises from the energy-conserving transitions of second and higher order perturbation diagrams. Numerous microscopic calculations are in progress to determine this term [11]. It seems, so far, that no convenient picture has emerged from such studies. Consequently, in order to carry out evaluations, one must still keep the absorptive part of the potential phenomenological. Recently, a non local energy dependent imaginary optical potential for s-wave neutrons incident on <sup>208</sup>Pb, has been calculated in the intermediate structure model with particle-vibration coupling [20]. This study succeeded in reproducing rather well the experimental resonances in absorption cross-sections below 2.6 MeV. Similar treatments may be expected to be used for practical purposes.

Let us note also the extensive attempts to construct transition

matrices for inelastic scattering. Use is also made of bound state two-body effective interactions, especially by SATCHLER [21]. In these studies, a folding model such as (6) is commonly used, in which a deformed target density is folded with a chosen effective two-body interaction expanded in multipoles.

# 2.3.3. The target wave functions

They are vibrational or rotational model wave functions. They occur in the non-radial parts of the potential matrix elements, which have simple analytic expressions [13]. When deformation parameters have negligible strength, inelastic channels are no longer coupled : this is the spherical optical model.

# 2.3.4. The common optical deformed potential

One assumes that the optical potential is the same for all the channels [15].

For neutron scattering, the optical potential can be written as :

$$U = -V_{R}f(r,R,a) - iW_{V}f(r,R_{V},a_{V}) + 4iW_{D}\frac{d}{dr}f(r,R_{S},a_{S})$$
  
+ 2V<sub>SO</sub>  $\chi_{\pi}^{2}\frac{1}{r}\frac{1}{dr}f(r,R_{SO},a_{SO}) \stackrel{\rightarrow}{\varUpsilon}_{.S},$  (7)

where :

-  $V_R$ ,  $W_v$ ,  $W_D$  and  $V_{so}$  are, respectively the real central potential, volume and surface absorption, and spin-orbit potential;

-  $\chi_{\pi}$  is the pion Compton wave length. It is a relic of the optical potential derivation from the meson field theory of nuclear forces. For evaluation purposes, the deformation parameters included in the spin-orbit term are usually neglected.

-  $f(r,R_i,a_i) = [1 + \exp(r - R_i)/a_i]^{-1}$ - the radius  $R_i$  can be expressed as :

 $R_{i}=R_{oi}\left[1+\sum_{\lambda\mu}\alpha Y^{\mu}(\widehat{\Omega})\right] \qquad \text{for vibrational nuclei, and}$ 

 $\begin{array}{ll} R_{i}=R_{oi}\left[1+\Sigma \ \beta \ Y^{O}\left(\theta'\right)\right] & \text{for axial-symmetric rotational nuclei} \\ \text{in the body fixed system with, in both cases :} \end{array}$ 

$$R_{oi} = r_{oi} A^{1/3}$$

- For rotational nuclei,  $\beta_{\lambda}$  is a permanent deformation parameter ( $\lambda = 2, 4, \ldots$ ), while  $\alpha_{\lambda\mu}$  is related to  $\beta_{\lambda}$ , for vibrational nuclei, through the relation :

$$\alpha_{\lambda\mu} = \beta_{\lambda}(2\lambda + 1)^{-1/2} \left[ b_{\lambda,\mu} + (-1)^{\mu} b_{\lambda,-\mu}^{+} \right]$$

where  $b_{\lambda,\mu}(b_{\lambda,\mu}^+)$  are destruction (creation) operators of one phonon states.

In order to obtain coupled equations, the optical potential is generally expanded in a diagonal part  $U_{\rm d}$  and in a non-diagonal part  $U_{\rm cp}$  .

For vibrational nuclei, the potential is expanded in a Taylor series of the deformation parameters, while, for rotational nuclei, it seems better to expand it in Legendre polynomials. As a consequence,  $U_d$  is deformation dependent (independent) for rotational (vibrational) nuclei.

Then, the coupled equations can be expressed as :

$$\begin{bmatrix} \widetilde{T}_{c} - E_{c} + U_{d} \end{bmatrix} u_{c}^{J\pi} = - \sum_{c}, \ <\phi_{c}^{J\pi M} \mid U_{cp} \mid \phi_{c}^{J\pi M} > u_{c}^{J\pi},$$

If one writes the coupling potential in the following way :

$$U_{cp} = \Sigma U(r,\beta) (Q(\beta).Y),$$
  
$$\Lambda \neq 0 \Lambda \Lambda \Lambda \Lambda$$

the matrix elements of  $U_{cp}$  have simple expressions. As an example, let us consider the  $0^+ - 2^+$  (ground state - one phonon state) coupling. Then, the reduced matrix element of  $Q_{\Lambda}$  is nothing more than the quadrupole deformation parameter  $\beta_2$ :

$$<0^{+} ||Q_{\Lambda}||2^{+} = \beta_{2} \delta_{2,\Lambda}$$
,

and  $U_{\Lambda}$  is  $\beta$ -independent. For rotational nuclei, it is different :  $U_{\Lambda}$  depends on  $\beta$ , and  $Q_{\Lambda}$  is  $\beta$ -independent. Let us consider two states  $|I^{\pi K}\rangle$  and  $|I'^{\pi K}\rangle$  of the ground state rotational band and the  $Q_{\Lambda}$  reduced matrix elements; these can be expressed as :

<  $I^{\pi K} ||Q_{\Lambda}|| |I'^{\pi K} >= (2I'+1) (I'\Lambda KO |IK)$ , with the usual notation for Clebsh-Gordan coefficients.

# 2.3.5. Adiabatic approximation

For rotational nuclei, when it is possible to neglect the energy of excited states - compared to the incoming neutron energy - it may be convenient, essentially for saving computer time, to use the so-called adiabatic approximation [13]. The scattering problem is there considered in the body-fixed coordinate system and subsequently the scattering wave functions are projected in the C.M. coordinate system. When this approximation is used, the levels of the ground state rotational band are automatically coupled.

#### 2.4. Calculated observables

The solution of the coupled equations leads to energy-averaged collision matrix S and to cross sections. Thus, in evaluation work, one may calculate :

. Shape elastic cross sections  $(\sigma_E)$  which are related, at very low energy, to potential scattering radii R',  $(\sigma_E \simeq 4\pi R'^2)$ ;

. Differential shape elastic, and direct inelastic cross sections  $(\sigma_{DT})$ , and polarizations ;

- . Absorption cross sections  $\sigma_{CN}$
- . Total cross sections  $\sigma_{\rm T}$  =  $\sigma_{\rm E}$  +  $\sigma_{\rm DI}$  +  $\sigma_{\rm CN}$

Compound elastic and inelastic cross sections can be obtained otherwise (cf. statistical model calculations) by the intermediate of generalized transmission coefficients  $T_c^{J\pi}$ :

$$T_{c}^{J\pi} = 1 - \Sigma_{c}, \quad S_{cc'}^{J\pi^{*}}, \quad S_{cc'}^{J\pi}, \quad (c,c' = open channels).$$

In the low neutron energy range (a few keV), the absorption cross section can be expressed in terms of neutron strength functions, which are related to the transmission coefficients.

$$S_{\ell} = \frac{1}{2\pi} \sqrt{\frac{E_0}{E}} \frac{1}{P_{\ell}} \left[ \frac{(\ell+1)T_{\ell}, j=\ell+1/2 + \ell T_{\ell}, j=\ell-1/2}{(2\ell+1)} \right], \quad (\ell=0, 1)$$

where  $P_{\ell}$  is a penetrability factor whose value is 1 if  $\ell = 0$ , and  $(kR)^2/[1+(kR)^2]$  if  $\ell=1$ . k is the wave number, and  $E_0$  a reference energy (1 eV is usually chosen).

These quantities are determined from resonance cross section analysis (R-matrix theory), with the following definition :

$$S_{\ell} = \frac{\langle \Gamma_n^{(\ell)} \rangle}{\langle D^{(\ell)} \rangle} \qquad (\ell = 0, 1) ,$$

where  $\langle \Gamma_n^{(l)} \rangle$  and  $\langle D^{(l)} \rangle$  are respectively the usual notations for average reduced neutron resonance width, and average resonance level spacing.

It appears that  $S_0$ ,  $S_1$  and R' can be considered as basic data for determination of the optical potential parameters. This is explained in the subsequent chapters.

#### 3.1. Conventional numerical methods

#### 3.1.1. Numerical integration methods

A review of the methods used in optical model calculations, with discussion of errors arising during the numerical integration of the radial Schrödinger equation, was very clearly reported by MELKANOFF and coworkers [2]. KIKUCHI [23] has made a comparison of numerical results obtained using the following optical model codes : MAGALI [24], GENOA [25], KOUAC [26], ABACUS2 [27], JUPITORI [28], ECIS 70 [29]. He proposes standard values of C-matrix coefficients, total cross sections, strength functions, differential elastic cross sections and polarizations, very useful for testing an optical model code.

A comparison of algorithms for the solution of coupled second order differential equations was made in a lecture given at the ICTP a few years ago by RAYNAL [30]. Comparisons were made between COWELL, NUMEROV, modified NUMEROV and DE VOGELAERE methods. Coupled-channel calculations are also used in Atomic Physics and we suggest the eventual possibility of applying their techniques in Nuclear Physics (see Allison [31], or [32] for example). For direct numerical integration of coupled equations, it seems to us that the modified NUMEROV method is the most appropriate. It permits the use of a larger radial mesh and requires less storage than the STORMER method. The direct solution of sets of coupled differential equations remains however a time consuming and expensive work. Thus, an iteration procedure has been developed by RAYNAL [30]. This "sequential iteration method" is used in the computer code ECIS. The convergence of the iteration procedure is very quick when the effect of the coupling is not too strong. For usual values of the quadrupole deformation parameter ( $\beta_2 = 0.2, 0.3$ ) of heavy nuclei, the effect of coupling is decreasing as the energy of the projectile is increasing, thus, we think that the convergence of such an iteration procedure depends on the energy of the projectile (quick at high energies, and perhaps not convergent at low energy).

Comparisons of numerical results of coupled-channel calculations were made by KIKUCHI [23]. In this reference one can find numerical values obtained from various computer codes : JUPITOR 1, ECIS 70, ADAPE [33]. We point out that numerical values obtained using hexadecapole deformation parameters are erroneous (due to a mistake in the input).

#### 3.1.2. Computer codes and their utilization

In discussing the use of computer codes in practical neutron nuclear data evaluation, we cannot mention here all optical model or coupled-channel codes. We choose some of them which have been used in evaluation works, or which present very interesting methods.

Standard optical model codes have an automatic parameter search subroutine which permits one to obtain a "best set" of parameters for <u>one</u> energy and <u>one</u> nucleus. Often, in an evaluation, we need a global set of parameters which covers a wide energy range. Using PEREY's code GENOA, it is possible, from simultaneous fits to several experimental data sets (angular distribution, total cross section) at various energies and for various nuclei, to obtain a global optical model parameter set. This code was used by FU and PEREY in an evaluation of neutron data for lead isotopes [34].

There are several computer programs for carrying out coupled-channel calculations. We shall discuss some of them.

The first and simplest ones are those which assume the coupling of the ground state  $(0^+)$  to the first excited level  $(2^+)$  of rotational or vibrational even-even nuclei, for example "2 PLUS" [35a]. In this computer code, the potential is expanded in powers of  $\beta$  up to the first order. Compound nucleus calculations are included : penetrabilities for the ground state and first excited level are calculated with a deformed potential whereas penetrabilities for higher levels are calculated with a spherical potential. Application of this formalism was made by DUNFORD [35b] in a study of neutron scattering from Ti, Fe, Zr. For evaluation purposes, this computer code was extensively used for heavy deformed nuclei by its author [35c] and more recently at Argonne [36].

A second group of coupled-channel computer codes is formed by the original or modified versions of JUPITOR1[28]. This program presents a great flexibility. It permits the coupling of up to five excited levels to the ground state, with a great variety of collective wave functions. The formalism used is very well described in[13]. Thus it was very easy to modify it, and many modified versions are used. We will mention some of them. The modified version adopted at [37] Karlsruhe by REBEL and SCHWEIMER is written in FORTRAN IV and works on the IBM 360 computer (the original version was written in "CDC FORTRAN 63"). In "JUPITOR KARLSRUHE VERSION" the double precision mode is used and an automatic search routine has been added. A detailed explanation of the modifications and tests is clearly presented in the report [37].

Other versions of JUPITOR-1 are currently used by PRINCE at Brookhaven and TANAKA at JAERI [38].

At Bruyères-le-Châtel, we make use of a "special" version : we have modified the algorithm used in the integration of the radial Schrödinger equation and adopted the modified NUMEROV method ; we have changed the output so as to obtain all the numerical data needed for evaluation purposes, in particular generalized penetrabilities, on punched cards ; the structure of the code has been modified to take advantage of a very useful overlay procedure.

Finally, a third group of computer codes making use of special techniques to reduce computing time should be mentioned. An example is ADAPE "A fortran program for the adiabatic coupled-channel calculation of nuclear particle scattering by rotational nuclei" of FABERI and ZUFFI [33]. This code was used to study the effect of nuclear deformation on the neutron scattering angular distribution with application to <sup>239</sup>Pu in an energy range 0.2 - 5.5 MeV [40]. The coupledchannel calculation code ECIS, which seems to us to be the quickest, has been used mostly for charged particle studies (angular distribution and analysing power). Its last version contains an automatic parameter search routine as well as options to introduce various collective wave functions, or to use a folding model for composite particles [41].

Other comparisons or descriptions of optical model computer codes are presented in contributed papers CP7 and CP11 at this Meeting.

#### 3.2. Matrix methods

It may be desirable, instead of numerical integrations, to use matrix methods for solving the Schrödinger equation describing the neutron scattering from an optical potential. For example, in the framework of the so-called "calculable R-matrix" method [42,43], variational forms of the phase-shifts can be obtained [44] which involve the inversion, at an energy E, of an A matrix whose elements are of the form :

$$A_{ac} = \langle a \mid T + U + a' - E \mid c \rangle \tag{8}$$

T, U and  $\varkappa$  represent, respectively, the kinetic energy, the potential, and the boundary condition operator of BLOCH [45]. In (8), the space-coordinate integration is performed within an internal region.

In the reference [46], the possibility has been examined to calculate the phase-shifts and scattering wave-functions from a neutron non-local spherical optical potential by using this method. The base states ( $|a\rangle$ ,  $|c\rangle$ ,  $\cdot \cdot$ ) used to expand the scattering wave function in the internal region ( $r \leq R_{max}$ ) are harmonic oscillator eigen-functions. For practical purposes, the phenomenological potential U was generated by a folding procedure with a Gaussian function v as in (6). Namely, the complete local form of U is written as :

$$U(r) = - \mathbb{V}_{R} \mathcal{V}_{R}(r) + 2\lambda_{\pi}^{2} \mathbb{V}_{so} \cdot \frac{1}{r} \cdot \frac{d\mathcal{V}_{so}(r)}{dr} \cdot \vec{k} \cdot \vec{s} - i\mathbb{W}_{V} \mathcal{V}_{V}(r) + i\gamma \mathbb{W}_{D} \frac{d\mathcal{V}_{D}(r)}{dr}$$
(9)

where the different functions  $\mathcal{P}(\mathbf{r})$  have the folding form (6). For example :

$$\mathcal{V}_{i}(r) = (\pi^{3/2} \cdot \mu_{i}^{3})^{-1} \int_{0}^{R} \exp \left[ |r-r'|^{2} / \mu_{i}^{2} \right] \cdot 4\pi r'^{2} dr' \qquad (R_{i} = r_{oi} A^{1/3})$$

$$(i = R, so, V, D) \qquad (10)$$

It has been shown in ref. [46] that the construction of the

matrix elements (8) including such a potential, is very practical when using the separable expansion of the Gaussian function v described recently by GOGNY [47] in the framework of H.F.B. calculations. This matrix method can be extended without any difficulty [46] to non-local potentials as defined, for example, in ref. [48]. Furthermore, it allows to calculate, in a single computer run, the derivatives of all phase-shifts, and consequently of all required cross-sections, with respect to all potential parameters and neutron energy. Many matrix calculations are, moreover, carried out once and for all when the various potential depths or the neutron energy are varied (see (8)). Thus, concerning the determination of best parameters, this matrix method is easier than the common numerical integration procedures. Fig. 1 shows in several typical cases, that the convergence obtained for the calculated phase-shifts (and cross-sections) as a function of the order of the A matrix (8), is reasonable even for heavy targets.

It is worth while to note that such methods may use real matrix elements  $\langle a | Re | u | c \rangle$  resulting directly from H.F.B. calculations. In this case, Re U is the better, non-local, single particle field.

Applications and extensions of the above method to evaluation purposes are in progress at Bruyères-le-Châtel.

# 4. EXAMPLES OF OPTICAL MODEL UTILIZATION FOR NEUTRON DATA EVALUATION PURPOSES.

A very large number of experimental data has been analysed using some selected forms of the spherical or deformed optical potential. These analyses have generally led to reasonable optical-model parameter sets. In the opposite way, these parameter sets are often used for neutron data evaluations. We shall mention here only a few examples of such typical or recent analyses, and commenton their utilization for evaluation purposes. In this context, it is convenient to distinguish between them according to the number of nuclei and the energy range, which are taken into account by a unique average parameter set.

#### 4.1. Local determination

A first kind of analyses contains "punctual" ones : these consist, for example, in a separated interpretation of the measured differential elastic and inelastic scattering cross sections for one nucleus at a given energy. Such data were, so far, probably the most frequently analysed. They are, however, directly comparable to calculations only at energy high enough ( $E \ge 5$  MeV), where compound processes are generally negligible. Such typical "punctual" analyses have been performed by HOLMQVIST and WIEDLING using measurements of elastic scattering angular distributions. In Fig. 2a are shown the parameter=search results obtained for many natural elements, from Al to Bi at 8 MeV neutron energy [49]. These spherical potential parameters exhibit fluctuations versus the A mass number. Nevertheless, they can be considered as useful ones for evaluations of scattering data (and, to some extent, for total cross sections) but in a limited energy range. On the other hand, shows the smooth energy variations of the parameters which Fig. 2b may be interpolated for evaluation of neutron data for Cu [50]. Some of the problems in optical model analyses of scattering data about parameter ambiguities and, especially about absolute normalization, are illustrated in PEREY'S recent review article [51]. The best-fit parameters to a single angular distribution may be inadequate for generating transmission coefficients needed in the analyses of various compound nuclear reactions. A compilation of optical parameters, determined from fits to elastic scattering angular distributions, was published [52].

#### 4.2. Average parameter sets

A second sort of analyses using spherical potentials consists in systematic parameter studies over a large range of energies and nuclei. Obviously, such a procedure leads to average parameters, with smooth energy and mass number dependences. Perhaps the most recent and widely used among these average sets of optical model parameters is the one determined by BECCHETTI and GREENLEES [53]. It is applicable to A > 40and determined on the basis of neutron data up to 24 MeV, and it is shown, with the notation of (7), in <u>Table 1</u>. Below 14 MeV neutron energy, the more adequate standard set, proposed by WILMORE and HODGSON [54], has been obtained as a local equivalent potential to the non-local potential of PEREY and BUCK [ 48 ]. This standard has been used extensively in Hauser-Feshbach calculations.

The usefulness of such standard optical potentials for the actual neutron data evaluations seems however to be relatively limited. Taking into account the accuracy generally required for many cross sections, these average parameters can only be used as a first approximation (for example as starting values in fitting procedures). Thus, in evaluation work, we are concerned with the extent of the departures from such global determinations, as discussed for example in ref. [55]. The spherical non-local potential of PEREY and BUCK [48] has been recently used by FOSTER and GLASGOW [56] in an analysis of their extensive neutron total cross section measurements of a number of nuclei ranging from hydrogen to plutonium in the energy range 2.5-15 MeV. The fit is generally good for spherical nuclei, but some strong discrepancies (about 6 times the experimental uncertainties) appear for deformed nuclei. These discrepancies may be considered as the effects of nuclear deformations.

Extensive coupled-channel calculations of total cross sections from 2.5 MeV to 15 MeV, and scattering cross sections at 8 MeV and 14 MeV, have been recently performed by TANAKA [57] over a wide mass number range. The potential parameter set has been determined from fit to neutron data of <sup>209</sup>Bi (spherical nucleus). The results obtained using C.C. formalism are always better than those resulting from a spherical optical model. Moreover, the effects of C.C. calculations are stronger at low energies. Despite the relatively good agreement obtained, the extrapolation of the TANAKA parameters to very low or high enough energies is not recommended.

#### 4.3. Local and adapted systematics

For evaluation purposes, it is probably more appropriate to use parameter sets which have been determined systematically over a small range of nuclei. In such cases, it is desirable to take into account the maximum of the available data in the region of interest in order to define the best physical parameters. In particular, the imaginary potential is expected to be carefully determined for transmission coefficient calculations. The potential used by MOLDAUER [58] is well suited for reproducing "s" wave strength functions as well as elastic scattering data below 1 MeV in the mass number 100 region . It is a good example of local and adapted systematics.

The pioneering work by DUNFORD [59] is a typical example demonstrating the utility of an appropriate comprehensive nuclear scheme for evaluation purposes. A coherent theoretical evaluation of several  $^{238}$ U neutron cross sections of interest has been performed over the full energy range from 10 keV to 15 MeV by using an unique adapted optical potential. In this work, however, the limited  $(0^+, 2^+)$  coupling mode was not able to provide as accurate results as now required.

Many similar analyses have more recently been attempted. Let us mention, for example, PRINCE's [60] evaluation of high energy neutron cross sections for a set of fissile and fertile isotopes. In order to describe the experimental data adequately, he used the C.C. formalism in which the first three levels were coupled, i.e.  $^{239}$ Pu  $(\frac{1}{2}^{+}, \frac{3}{2}^{+}, \frac{5}{2}^{+})$ ,  $^{241}$ Pu  $(\frac{5}{2}^{+}, \frac{7}{2}^{+}, \frac{9}{2}^{+})$  and  $^{240}$ Pu,  $^{238}$ U  $(0^{+}, 2^{+}, 4^{+})$ . The model parameters were chosen so as to satisfy four experimental constraints : the total scattering cross section, the potential scattering cross section, and the s and p wave strength functions. In this relatively more elaborate study, however, the nuclear radii had to be varied with the neutron energy so as to improve the fits. The satisfactory interpretation obtained by BENZI and coworkers [40] of  $^{239}$ Pu differential elastic scattering cross sections, measured in the

- 270 -

energy range 0.19-5.5 MeV, is an example of the utility of using an adapted theoretical frame. In this case of an odd target, he assumed that at low energy all the excited states up to the  $(\frac{7}{2}+)$  level had to be strongly coupled with the ground state. As a result of such a realistic but time-consuming treatment, it was possible to adopt parameters which are similar to those successfully used for neighbouring nuclei and, consequently, more convenient for extrapolations.

Several attempts for understanding physical aspects of 0.M.parameterisations have been done, in the last few years, by analysing various experimental cross sections for an isotopic chain. An example of such investigations, intended to evaluation purposes, is the analysis by SMITH and coworkers [61] of neutron total cross sections for 92, 96, 98, 100 Mo measured from 1.6 to 5.5 MeV, and neutron elastic and inelastic scattering cross sections for the same isotopes measured from 1.8 to 4.0 MeV. One of the main objectives of such studies is to improve our understanding of the optical model parameters in well defined mass number regions where the possible influence of particular nuclear structure effects has to be carefully investigated.

#### 4.4. The "SPRT" method

In the method used at Bruyères-le-Châtel for the determination of optical potential parameters over a wide neutron energy range (a few keV up to 20 MeV, and more), the "s" and "p" wave strength functions  $(S_0 \text{ and } S_1)$  and the potential scattering radius (R') are considered as base data. One takes into account also, on the same footing, the energy dependence of the total cross section  $\sigma_T$  (E) because it is the only cross section for which the energy averaged measurement is directly comparable to optical model calculations over the full energy range.

In a first approximation, the spin-orbit potential  $V_{so}$  is chosen to have standard strength and geometry. Small deviations from these values have negligible effects on  $S_1$  and, sometimes, larger effects on  $\sigma_T$ .  $V_{so}$  is improved later in its shape and strength when the imaginary and central real potentials are determined.

For a given nucleus, an optical potential parameter set is considered as promising if it leads to acceptable values for  $S_0$ ,  $S_1$  and R'

calculated at low neutron energy (10 keV for example). This parameter set is then used to compute the  $\sigma_{\rm T}$  smooth energy variations up to few MeV (10 MeV for example) when the competition between the surface and the volume absorption is still negligible. From the analysis of  $\sigma_{\rm T}$ , one can extract the energy variations of V<sub>R</sub> and W<sub>D</sub>. This analysis of the minima, maxima, and the shape of gross structures in  $\sigma_{\rm T}$  is a crucial step, and one must be prepared to continue searching for new sets of optical potential parameters <u>as long as it is necessary</u> to obtain reasonably good calculated values for S<sub>0</sub>, S<sub>1</sub>, R' and to reproduce the energy dependence of  $\sigma_{\rm T}$ .

Using the final parameters set, at energies for which compound effects are negligible, the calculated elastic scattering angular distributions generally have shapes close to corresponding experimental values. The same conclusion has been verified also while using the folding potential for spherical nuclei.

The agreement can be improved (especially at backward angles) if the spin-orbit potential is slightly changed from the shape and strength chosen originally. Moreover, so as to be sure that the surface absorptive potential  $W_D$  has a good energy variation, one has to compare the calculated and the experimental direct inelastic cross sections, and change  $W_D$  if necessary. None of the optical parameters was determined by least-squares fitting procedures.

At higher neutron energies, between 10 MeV and 20 MeV, there are generally not enough accurate measurements of angular distributions and reaction cross sections. For this reason, it is difficult to determine the competition between the surface and the volume absorption. However, a study of proton scattering cross sections could be useful for its determination.

Using this "SPRT" method, a number of nuclei have been studied[62, 656869] over a wide mass number range (A = 89 to 238) in term of spherical, vibrational and rotational models, using various coupling schemes. Some examples of so calculated strength functions ( $S_0$  and  $S_1$ ) and potential scattering radii (R') are given and compared to their experimental values in <u>table 2.</u> In all cases which have been studied so far at Bruyères-le-Châtel, it was always possible to get, from this method, acceptable parameterisations. In particular, we have never met any impossibility to obtain reasonable  $S_0 \xrightarrow{and} S_1$  strength function values. Moreover, it is worthwhile to mention these simultaneous adjustments onto  $S_0$ ,  $S_1 \xrightarrow{and} R'$ were requiring no  $\boldsymbol{\ell}$ -dependence of the imaginary potential depths. 5. MAIN COMMON PROBLEMS IN OPTICAL MODEL CALCULATIONS

#### 5.1. Choice of the coupling scheme

Perhaps the most important aspect of coupled-channel calculations lies in the choice of the coupling scheme.

#### 5.1.1. Preliminary remarks

As neutron energies are increased from a few keV to several MeV, calculated values become less and less sensitive to the chosen coupling scheme. Nevertheless, this choice must be the same over the full energy range. In order to reduce the extensive computation time, it is possible, however, in the case of rotational nuclei, to change the coupling basis and adopt the adiabatic approximation when the energy of the projectile is high enough compared to the low-lying excitation energies. The radial factors of the coupling can be chosen complex or real. Since the effect of this choice is not the same for all calculated values (strength functions, total cross sections, scattering angular distributions) in the full energy range, one has to do a global analysis and decide, in each case, which is preferable.

# 5.1.2. Choice of a coherent basis

When calculations are done for an isotopic chain of nuclei, the coupling scheme must be physically coherent for all of them. For even isotopes, we recommend the choice of a coherent coupled-state basis in target spin space. Let us mention, for example, the case of the even Samarium isotopes. The first excited states for all these isotopes have the same spin and parity  $(I^{\pi} = 2^{+})$ , but the second excited states have differing values of  $I^{\pi}(3^{-}, 2^{+} \text{ and } 4^{+})$ . In a recent study [62], we have chosen the most simple and coherent coupling basis : ground state and first excited level  $(0^{+}, 2^{+})$ . For odd nuclei, the choice is not so clear. For all the rotational nuclei, we can use the adiabatic approximation at high energy and adopt equivalent bases for each of them at lower energies.

We notice that, for rotational and vibrational nuclei, the two bases  $(0^+, 2^+)$  and  $(1/2^+, 3^+/2, 5^+/2)$  are equivalent. For odd vi-

brational nuclei, the weak coupling model of de SHALIT [63] can be used as a guide for the coupling scheme. At Bruyères-le Châtel, in the framework of a first theoretical evaluation, we have judged it sufficient in the case of odd rotational nuclei to interpolate the results from the two neighbouring even isotopes.

# 5.1.3. Dimension of the coupling basis

There are two opposing views about the choice of the coupling basis : the first contends that coupled-channel calculations are useless and that spherical optical model calculations are sufficient. In this case, one assumes that direct inelastic scattering of neutrons from first excited states of collective nuclei is negligible. We now have evidence that in many instances this is not true (for not too small deformation parameter values). SMITH and coworkers [64] measured the elastic and inelastic scattering of 3 MeV neutrons from <sup>186</sup>W. The data and very preliminary calculations by DELAROCHE (the parameters were determined following the above so-called SPRT method) are shown in fig. 3a . The measured differential cross sections point out that inelastic scattering from the first excited level (2<sup>+</sup>, 123 keV) is comparable to or greater than elastic scattering at the minima of the elastic angular distribution and at backward angles. Theoretical calculations including compound process are in very promising agreement with experimental results. In these calculations, direct inelastic scattering processes contribute 75% of the total inelastic cross section for this level. When the energy resolution is not sufficient to resolve inelastic scattering to excited states belonging to the ground state rotational band, coupled-channel calculations give useful indications. The measured neutron differential elastic cross sections for <sup>148</sup> Sm and elastic plus inelastic scattering cross sections for <sup>154</sup>Sm and coupled-channel calculations ("SPRT" method) are shown in fig. 3b . It is clear that the assumption of negligible direct inelastic scattering may lead to think that the major effect of nuclear deformation on the elastic scattering is to increase the cross section at the minima of the elastic angular distribution. Coupled-channel calculations show that such a conclusion is probably erroneous. Measurements of inelastic scattering of neutrons from <sup>238</sup>U made by SMITH [65]

(see also fig. 9) have shown the importance of such couplings in this mass region.

The second point of view is that realistic coupled-channel calculations can only be done with a great number of coupled levels. It is well-known that, for a given parameter set, calculated values converge when the coupling basis is increased. But in coupled-channel calculations, the set of deformations and optical model parameters used depend on the number of basis states included. We think that, for a given nucleus, the choice of a great number of excited levels coupled to the ground state is not an absolute guarantee of success. For example, even though TANAKA [57] has used a large basis  $(0^+, 2^+, 4^+, 6^+)$  in his coupled-channel calculations of total and scattering neutron cross sections, the agreement with experimental data for the actinides is, in general, not very good. Our calculations for  $^{238}$ U [66] indicate that good agreement can be obtained using a smaller basis  $(0^+, 2^+, 4^+)$  and adjusting the optical parameters.

An intermediate position can be adopted between these two extreme view points. Criteria for the choice of the coupling scheme may come from considering neutron data at low energies and total cross sections over the full energy range. Since the determination of the optical model and deformation parameters is <u>not</u> independent of the choice of the coupling basis, one must be <u>wary</u> of <u>erroneous conclusions</u> based on parameterisations not realistic enough (optical model parameter set not physically coherent or coupling basis too much restricted).

#### Remark

Recent theoretical calculations of neutron data have been done for  $^{93}$ Nb approximately in the same energy range by TANAKA [57], SMITH [67], LAGRANGE [68]. The first one is a coupled-channel calculation based on the weak coupling model of de SHALIT (a proton and a vibrating core  $^{92}$ Zr), using the deformation parameter :  $\beta_2 = 0.11$ . The other two are spherical optical model calculations. In the three cases, the optical model parameters were different. This is a very good example of difficulty sometimes met in the choice of the coupling scheme. 5.1.4. Other example of the importance of the coupling scheme

The effect of the choice of the coupling scheme was shown in the particular case of <sup>238</sup>U by LAGRANGE [69]. The method used for determining the optical model parameters has been discussed previously as the SPRT method.

In a first approach, the ground state and the first excited state coupling scheme  $(0^+ - 2^+)$  was taken. Though quite a good agreement was obtained for  $S_0$ ,  $S_1$  and R' (cf. <u>table 2</u>), that was not the case for the total cross-section (cf. <u>fig. 4a</u>, 4b).

In a second approach, a larger coupling basis  $(0^+ - 2^+ - 4^+)$  was used, and very good agreement was obtained for the low energy neutron data (S<sub>0</sub>, S<sub>1</sub> and R') as well as for  $\sigma_{T}(E)$ .

The optical model parameters are different in each case. The effect of these two basis choices on the "elastic" angular distribution is shown in <u>fig. 4c,4d</u>. At these energies, the experimental resolution is not good enough to resolve inelastic scattering from the first two excited levels. We notice here that a good agreement between experimental and calculated scattering cross-sections was obtained without any new parameter adjustment.

#### 5.2. Determination of potentials

As in the case of the coupling scheme, the potentials chosen have to be physically coherent in the full energy range (a few keV to 20 MeV for example). We share with the Argonne Laboratory Group [70] the belief that "The potentials are specific to the given nuclei and not necessarily of a general nature", and we consider (as do they), the total cross section as base data for the determination of parameters. The choice of a coupling scheme and of a potential usually permits one to calculate total as well as direct scattering cross sections. But for an extensive theoretical evaluation in the full energy range, one needs transmission coefficients used for compound elastic and inelastic calculations at low energies, and for statistical cross section calculations at higher energies ((n,2n) for example).

Usual methods of determining the strength and energy variations

of the real and absorptive part of the potential, can be illustrated by the following example. TANAKA [57] determined the parameters of a spherical optical potential by fitting elastic data for  $^{209}$ Bi at various energies, and, so adjusted, the energy dependence of the real and imaginary well depth are shown in <u>fig. 5</u>. BENZI [71] has clearly demonstrated that the crude extrapolation to zero energy of potentials resulting from a global analysis of  $^{63}$ Cu neutron cross sections above 3.5 MeV, gives poor predictions of the inelastic scattering cross sections at low energies (see <u>fig. 6</u>). Thus, the choice of the absorptive and real part of the potential must be done carefully.

#### - Determination of the absorptive part of the potentials

At very low energies, the "s" and "p" wave strength functions are closely related to the compound nucleus formation cross section and thus to the absorptive part of the potential. Moreover, pioneering work of MARGOLIS and TROUBETSKOY [72] has shown the great sensitivity of strength functions to nuclear deformations. For these reasons, we think that a good fit to these experimental quantities may give with confidence the absorptive part of the potentials. The imaginary depth so obtained (3 MeV for example) at low energies, is less than that usually employed (9 MeV for example) at higher energies. This problem is usual in attempts to give a global description of neutron data over a wide range of energies. An increase in the strength of the absorptive part with neutron energy E was adopted by FU [34], BENZI [40], TANAKA [57], DUNFORD [35c], LAGRANGE [66]. In all cases, this absorptive part was peaked at the surface of the nuclei (derivative of a WOODS-SAXON form), and its strength was respectively (in MeV) : 3.5 + 0.43 E, 3.52 + 0.52 E,  $2.55 \sqrt{\text{E}}$ ,  $6.68 + 1.3 \sqrt{\text{E}}$ , 2.7 + 0.4 E. At high energies, volume absorption appears, and it is usual then to take an increasing volume absorption together with a decreasing surface absorption.

A decreasing energy dependence of the absorptive part over the full energy range, leads to unrealistic small values of compound nucleus formation cross sections at high energies. For example, the energy dependence of the absorptive part of the potential (WOODS-SAXON derivative form) chosen by SMITH [67] and coworkers for <sup>93</sup>Nb was

#### - Determination of the real part of the potential

The strength and energy variation of the real potential are much better known (see for example [8]) than those of the imaginary part. The depth of the real potential is generally decreasing with increasing neutron energies. This behaviour is usually determined by fitting elastic neutron cross sections. But, provided  $V_R r_o^n$  is taken constant (n = 2 or 3), with  $r_0$  values ranging from 1.17 to 1.35, several corresponding values of  $V_{R}$  can be found which give equivalent fits to the elastic data. As the shape elastic scattering cross section is related to the experimental value of the potential scattering radius (R'), we think that fitting these experimental data permits the determination of  $V_{\rm R}$ . The following example of applying the "SPRT" method to <sup>238</sup>U demonstrates clearly that employing such a procedure ambiguity. Calculated values of various <sup>238</sup>U Varn eliminates the for different combinations of potential parabasic neutron data meters are shown in table(3) along with recommended values of the ex-Results from the <sup>238</sup>U optical potential of perimental data. LAGRANGE [66] are shown in the third column, while the numbers in the second and fourth columns result from varying  $V_R$  and  $r_o$  such that  $V_{\rm R}r_0^2$  remains constant. In the fifth column,  $r_0$  was fixed at the value used in column 4 (1.17 fm), and  $V_R$  better adjusted to fit the recommended values of  $S_0$ ,  $S_1$ , and R'. The  $V_R r_0^n$  ambiguity is clearly removed by requiring simultaneous agreement with all the quantities listed in the table.

## 5.3. Isospin effects

A complete review article about isospin dependence of optical model potential was given recently by SATCHLER [74].

It has long been observed that, at the same energy, cross sections for neutrons and protons have different shapes and strengths, and that the nucleon-nucleus potential is more attractive for protons than for neutrons. Though this difference was partly explained in terms of the proton Coulomb field, it was shown, in analyses of proton scattering over a wide range of nuclei [75], that the proton optical potential contains a part whose strength is proportional to the asymmetry term: $\varepsilon = (N-Z)/A$ . A survey of neutron scattering from many nuclei [76] led to the same conclusion, but with the opposite sign for this asymmetry term.

One may write this dependence of the LANE optical potential, both for protons and neutrons, in terms of an isovector coupling [77] :

 $U(r) = U_{0}(r) + 4 U_{1}(r) \overrightarrow{t} . \overrightarrow{T}/A$ ,

where  $\vec{t}$  is the isospin of projectile, and  $\vec{T}$  the isospin of target.

In isospin space, the diagonal matrix elements can be expressed in terms of the asymmetry  $\boldsymbol{\varepsilon}$  :

$$< t_3 = \pm 1/2, T_3 = (N-Z)/2 |U|t_3 = \pm 1/2, T_3 = (N-Z)/2 > = U_0 \pm U_1 \epsilon$$

Moreover, U has non-diagonal matrix elements :

 $\langle f | U | i \rangle = \langle t_3 = +1/2, T_3 = (N-Z)/2 - 1 | U | t_3 = -\frac{1}{2}, T_3 = (N-Z)/2 \rangle = 2 U_1 (\epsilon/A)^{1/2}$ . It is supposed that the target lies in its minimum value for T :

$$T = T_3 = T_0 = A\varepsilon/2.$$

The transition amplitude < f |U| i > connects the ground state of the target  $|T = T_0, T_3 = T_0$  > to its analog  $|T = T_0, T_3 = T_0 - 1$  > in the residual nucleus (with N-1 neutrons and Z + 1 protons). Such (p,n) transitions where observed originally by ANDERSON and WONG [78], and are direct tests for the shape and strength of the isovector potential U<sub>1</sub>. An optical potential parameter set is "LANE consistent" if it is able to reproduce the following experimental results : (p,p), (n,n)cross sections as well as charge exchange (p,n) cross sections through isobaric analog state. Such studies are in progress [79,80].

Many experimental measurements were done for the determination of the isospin potential  $U_1$ . Most of them are related to proton scattering measurements [75] which are much easier to undertake than neutron experiments whose accuracies are generally not sufficient to determine optical potential parameters with any precision. Accurate measurements of the total cross section at high neutron energy (14.2 MeV) from many separated isotopes over a wide mass number range [81] led to  $V_1$  and  $W_1$  components of the LANE potential (respectively real and imaginary parts of  $U_1$ );  $V_1$  is smaller than usually found for proton experiments.

HOLMQVIST [82] obtained also a similar trend for V<sub>1</sub> from neutron angular distribution analysis below 8 MeV.

The global analysis by BECCHETTI of proton elastic scattering and polarisations was extended  $[7\vec{6}]$  to study neutron scattering between 1 and 50 MeV. The resulting optical potential is similar to that obtained for protons, but is not exactly "LANE consistent". This is, however, the most extensive study for neutron and proton scattering.

In the low energy range, there are other neutron data which seem to show evidence for a complex isospin potential."s" wave neutron strength functions have shown a remarkable systematic decrease with mass number A for each of many isotopic chains. In the mass region of Tin, Tellurium and Xenon [83], this trend is clear (see <u>fig. 7a</u>). This behaviour of S<sub>0</sub> with A is quite contrary to the predictions of the conventional C.C. optical model calculations which indicate a gradual rise for S<sub>0</sub> in this region [84].

The possibility that this effect is correlated with the asymmetry (N-Z)/A, was investigated for each isotopic chain. C.C. calculations were performed assuming a  $0^+ - 2^+$  vibrational coupling scheme for eveneven nuclei, except for <sup>130</sup>Xe which is considered to be a rotational nucleus. For even-odd Tellurium isotopes, to be coherent, a  $1/2^+ - 3/2^+ - 5/2^+$  vibrational coupling scheme is chosen. There is good qualitative and quantitative agreement between experimental results and calculations [83] if a complex asymmetry dependent potential is used (see <u>fig. 7a</u>). Recently, accurate measurements of neutron elastic and 2<sup>+</sup> inelastic angular distributions were performed [85] for even-even isotopes of the Selenium isotopic chain. Though the  $\beta_2$  deformation of <sup>76</sup>Se is known to be larger ( $\beta_2 \sim 0.28$ ) than that of <sup>82</sup>Se ( $\beta_2 \sim 0.17$ ), the experimental 2<sup>+</sup> inelastic cross sections have typically the same strength. It was shown [85] that the inelastic and elastic measured angular distributions are consistent with C.C. calculations if U<sub>1</sub> is taken to be complex. Experimental results and calculations are shown in <u>fig. 7 b</u>, for 8 MeV neutron energy.

These results can be probably considered as the first evidence of complex isospin effects in neutron elastic and inelastic scattering from isotopic chains.

As another test for U<sub>1</sub> determination, it has been suggested by LAGRANGE [86] that the calculated difference  $\frac{\Delta \sigma_{\rm T}}{\sigma_{\rm T}}$  of total cross sections for two neighbouring Samarium isotopes is very T sensitive to U<sub>1</sub> variations. When  $\frac{\Delta \sigma_{\rm T}}{\sigma_{\rm T}}$  is plotted versus the neutron energy, the point where the ratio crosses through zero strongly depends on U<sub>1</sub> (see <u>fig. 8</u>).

In the evaluation of neutron data, it is desirable to determine the isospin potential  $U_1$ . For a given isotopic (or isotonic) chain, we think that it is an important aspect of 0.M. calculations. The knowledge of LANE potential is indeed the simplest way to calculate cross sections even if experimental data are missing (Example : cross section determination for low isotopic abundance nuclei).

We think that the study of cross sections for an isotopic chain must begin with the isotope (s) for which a great number of experimental data is available. Then, it is possible to determine the geometry and the energy variations of potentials. When some ambiguities remain, it seems convenient to extend the study to proton scattering data.

There are other instances in which knowledge of the isospin potential is very useful : natural mono-isotopic element, as <sup>197</sup>Au for example. If one has to calculate neutron cross sections for the unstable nuclei of that isotopic chain, it is not possible to determine both optical potential and  $U_1$  from the single stable isotope neutron data. Thus, one must consider proton scattering data for this isotope and, if necessary, charge-exchange (p,n) cross sections [80]. When  $U_1$  is determined in such a way for this stable isotope, it is possible to know the optical potential for unstable nuclei of the isotopic chain through the LANE consistency.

#### 5.4. Target wave functions and form factors

In coupled-channel calculations, spectroscopic studies of nuclear structures guide us for the choice of form factors and coupling matrix elements. As usual, we shall distinguish between macroscopic and microscopic descriptions of nuclei.

# 5.4.1. Macroscopic description

In macroscopic description of nuclei, the individual orbits of the nucleons are neglected, and only the global collective motion is taken into account. The macroscopic models are mainly the rotational and vibrational ones. Such models are used in coupled-channel calculations, the interaction between the projectile and target nucleus is simulated with an optical potential including deformation parameters. Both of these extreme models are mostly used. The following example shows that some more sophisticated wave functions may be needed.

The Samarium isotopes are particularly appropriate for studying the collective nature of nuclei (they are in a transition region) : <sup>148</sup>Sm can be considered as a pure vibrational nucleus, and <sup>154</sup>Sm as a pure rotational one. The neutron total cross section for <sup>148</sup>Sm and total cross section differences for <sup>150</sup>, <sup>148</sup>Sm, <sup>152</sup>, <sup>148</sup>Sm and <sup>154</sup>, <sup>148</sup>Sm,from 0.7 to 15 MeV neutron energy, have been measured by SHAMU and co-workers [86]. Experimental results and coupled-channel calculations by LAGRANGE [86] are shown in <u>fig. 8</u>. Optical model parameters were adjusted so as to obtain (following the "SPRT" method) a good agreement for <sup>148</sup>Sm neutron total cross section. The knowledge of the isospin term was improved by considering 16 MeV proton scattering data.

Within coupled-channel calculations, one may see that a good agreement is obtained using the rotational model for  $^{152}$ Sm,  $^{154}$ Sm and the vibrational model for  $^{148}$ Sm. As for  $^{150}$ Sm, neither the vibrational model nor the rotational one can give a good agreement over the

full energy range.

The choice of deformation parameters seems to be very crucial. We have noted that at low energies, the global set of other parameters was very sensitive to deformation parameter values. Coulomb excitations, electron scattering and muonic x-ray experiments provide measurements of the deformation of the charge distribution, while a-particle, proton and neutron scattering experiments lead to the determination of nuclear potential deformations. It is usually assumed, however that the deformation parameters are independent of the excitation means, and so, could be taken in a bibliography [87]. Recently, MADSEN 88 has argued that deformation parameters extracted from various experiments could depend on excitation. In the case of an isotopic chain of nuclei, the choice of a deformation parameter set must be coherent for all nuclei. For these reasons and because of large experimental errors associated with their measurements, the use of deformation parameters issued from a common nuclear model is expected. For deformed nuclei, we may employ the NILSSON model and the methods of STRUTINSKY, as described by MÖLLER [89].

# 5.4.2. Microscopic description

As previously explained, the common phenomenological collective models may fail, and it seems that improvements are desirable for them. In an other way, the excited states can be determined through a microscopic point of view, whose interest lies in the unified description of collective and non-collective excited states. Many of such microscopic theories are in progress for inelastic scattering of nucleons (but especially for protons and high energies) from deformed nuclei. Let us here quote only some of them.

A CC-formalism including microscopic wave-functions was given by GLENDENNING [15] with a few applications [90]. SEVGEN [91] develops a R-matrix type theory for permanently deformed nuclei. Within the framework of the Distorted Wave Born Approximation (DWBA), SCHAEFFER [92] built a formalism which includes microscopic excited wave functions and antisymmetrisation effects. Many other references to important studies about this subject can be found in the SHINA's review paper [11]. These microscopic approaches of inelastic scattering were not used in the evaluation of neutron scattering data. However, they could be instructive ones, especially for non-collective and complex collective low-lying excited states of some nuclei (for example, in shape transitional regions).

#### 5.5. Transmission coefficients

The transmission coefficients (TLj) can be calculated from the appropriate optical potential and included in calculations of various compound nuclear cross sections : elastic, inelastic to each excited level of the target, radiative capture, (n,2n), (n,3n), fission.... These cross sections appear to be rather sensitive to the choice of transmission coefficients, especially for small 1-values, or near the reaction threshold energies. Consequently, the choice of the appropriate optical potential must be carefully taken (in particular for the imaginary part). It is recommended, in such cases, to use parameter sets obtained from fits to "primary data" : So, Sl. Moreover, a good energy dependence, at least at low energy, of the potential strengths has to be chosen so as to obtain realistic excitation funtions. An example of the extent to which inelastic scattering cross sections from low-lying excited levels depend on the choice of the optical model, is given in Fig. 6. Three HAUSER-FESHBACH calculations, including the width fluctuation effects as described by MOLDAUER, of the inelastic scattering from the first  $2^+$  excited state of  $^{238}$ U, are shown in Fig. 9. We have therein used two spherical potentials adjusted on (i) <sup>238</sup>U total cross-sections [93], and (ii) elastic and inelastic scattering from the lead isotopes [34]. The third calculation, a coupled-channel one, using the LAGRANGE's parameters [66], gives a compound component comparable to that resulting from the calculation (ii) and a direct component which predominates at energies higher than 1.5 MeV. In these calculations, we have not taken into account possible correlations between the reduced neutron widths for the entrance channel and the exit channel [94]. More details about <sup>238</sup>U coherent theoretical evaluations between 3 keV and 20 MeV, may be found in Ref. [95].
Simplified statistical model calculations need only the compound nucleus formation cross-section  $\sigma_{\rm CN}$ . For example, fission cross-section estimations may be obtained as  $\sigma_{\rm CN}$  times the measured fission probabilities P<sub>f</sub> of residual nuclei resulting from such direct reactions as (d,p), (t,p)... [2]. More generally, another example is given by statistical models excluding the total angular momentum and parity conservation rules. Such a treatment has been used in Ref. [96] for evaluating (n,2n), (n,3n) and fission cross-sections for a set of uranium and plutonium isotopes. In Fig. 10(a) and 10(b) are shown calculations of  $\sigma_{\rm CN}$  for <sup>238</sup>U which used the same three parameter sets as those in Fig. 9. It is clear that a careful theoretical treatment is needed especially at low energies.

## 6. CONCLUSIONS. PROSPECTIVES AND SUGGESTIONS

With the increase in the number and precision of the experimental data on the one hand, and with the progress of the microscopic view on nuclear structure on the other hand, it will be increasingly possible to distinguish between the various components of the optical model and to have a better knowledge of their behaviour as a function of the energy and mass number. It is true that a more detailed consideration of the phenomenological optical potentials leads to an increasing number of parameters. Microscopic analyses which relate to a wide range of various physical phenomena, and the fitting of more extensive and accurate sets of experimental data, may however, be helpful for assigning to those parameters more realistic expressions. In this context, it is worth while to note that the use of Hartree-Fock-Bogoliubov (H.F.B.) single particle fields, for example in the practical form of matrix elements, as described in Chapter 3, would provide a real part of the optical potential without any free parameters. It is not unrealistic to expect that in not too distant a future, complete but practicable H.F.B. calculations, such as those carried out recently by GOGNY [19], will thus be able to help in this sense the evaluation work for sets of important and or not easily accessible nuclei, e.g. transactinium nuclides or unstable fission products. On the other hand, taking into account present-day difficulties to calculate the imaginary potential using microscopic methods, this term of the nucleon-nucleus interaction would have to retain its phenomenological aspect.

At this moment however, it can be hopefully felt that recent efforts carried out in several laboratories for obtaining a reasonably coherent parameterisation of the potentials, will open the way to more reliable evaluations. While there is now agreement in some areas, there is much that still remains to be done in the determination of optical potentials suited for evaluating energy-averaged cross sections for a given nucleus over an energy range from a few keV to 20 MeV. Obviously, this progress in our understanding of the optical model has to be closely associated with the progress of other reaction models (statistical, preequilibrium, fission...) discussed at this Meeting.

Considering that the evaluation work is related to many and various cross sections over a wide energy range, it is important to

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improve the methods for the determination of optical model parameters. This improvement leads to optical potentials reflecting more and more physics, especially nuclear structure. Attempts towards this direction were undertaken but were not yet completely successful for all the nuclei to be studied. In particular, we think that one must give up the rough idea of a unique optical potential geometry valid for many nuclei. It seems, however, possible to determine a physical and consistent geometry well adapted to a small number of neighbouring nuclei (an isotopic chain for example) if a few experimental data are taken as strong tests :  $S_0$ ,  $S_1$ , R' and the energy variation of  $\sigma_{T}$ . Such fundamental experimental constraints in the parameter search allow to have a high level of confidence in the physical meaning of the obtained potentials, to do some interpolation and or extrapolation if necessary. We consider, thus, an important request to have, at low neutron energy, systematic and more accurate data, i.e. p-wave neutron strength functions. The imaginary part of the optical potential, between about 10 and 20 MeV, could be determined with reasonable precision under the condition that at least the elastic angular distributions are extensively measured. As a consequence, it should be possible to determine with more confidence other cross sections ((n,2n) for example) in the framework of the statistical model.

Though it is nice to foresee the possibility of determining the geometry of physically meaningful optical potentials with enough accuracy, such a determination has to be made in each particular case. Of course, this procedure is slower and more time consuming, but also more realistic.

As regards the theoretical tools and information, there is a general lack of systematic and accurate knowledge of quantities such as form factors and deformation parameters. It would be desirable to obtain such information independently of the evaluation work.

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REFERENCE	OPTICAL POTENTIAL PARAMETERS
(a) SPHERICAL NUCLEI [53]	$\begin{split} & \mathtt{V}_{\rm R} = 56.30 - 0.32 \ \mathtt{E} - 24(\mathtt{N-Z})/\mathtt{A}; \ \mathtt{r}_{\rm o} = 1.17; \ \mathtt{a} = 0.75 \\ & \mathtt{W}_{\rm v} = 0.22 \ \mathtt{E} - 1.56 \ ({\rm or \ zero}, \ {\rm whichever} \ {\rm is \ greater}) \\ & \mathtt{W}_{\rm D} = 13.00 - 0.25 \ \mathtt{E} - 12 \ (\mathtt{N-Z})/\mathtt{A} \ ({\rm or \ zero}, \ {\rm whichever} \ {\rm is \ greater}) \\ & \mathtt{r}_{\rm oD} = 1.26; \ \mathtt{a}_{\rm D} = 0.58 \ ; \ \mathtt{r}_{\rm ov} = \mathtt{r}_{\rm oD}; \ \mathtt{a}_{\rm v} = \mathtt{a}_{\rm D} \ . \\ & \mathtt{V}_{\rm so} = 6.20; \ \mathtt{r}_{\rm oso} = 1.10; \ \mathtt{a}_{\rm so} = 0.75 \ . \end{split}$
(b) 238 <sub>U</sub> (0 <sup>+</sup> -2 <sup>+</sup> -4 <sup>+</sup> ) [66]	$V_{R} = 47.50 - 0.30 \text{ E} \text{ ; } r_{o} = 1.24\text{; } a = 0.62$ $W_{v} = 0$ $W_{D} = \begin{cases} 2.70 + 0.40 \text{ E} (\text{E} \le 10 \text{ MeV}) \\ 6.70 \qquad (\text{E} > 10 \text{ MeV}) \end{cases} r_{oD} = 1.26\text{; } a_{D} = 0.58$ $V_{so} = 7.50\text{; } r_{so} = 1.24\text{; } a_{so} = 0.62$
(c) 89 <sub>Y</sub> SPHERICAL NUCLEUS [68]	$V_{R} = 49.50 - 0.28 \text{ E; } r_{o} = 1.24; \text{ a} = 0.62$ $W_{V} = 0$ $W_{D} = \begin{cases} 3.40 + 0.30 \text{ E} (\text{E} \le 8 \text{ MeV}) \\ 5.80 \\ (\text{E} > 8 \text{ MeV}) \end{cases} r_{oD} = 1.26; a_{D} = 0.58$ $V_{so} = 6.20 \text{ ; } r_{oso} = 1.12; a_{so} = 0.47$
(d) 93 <sub>Nb</sub> SPHERICAL NUCLEUS [68]	$V_{R} = 49.50 - 0.28 \text{ E; } r_{o} = 1.24; \text{ a} = 0.62$ $W_{V} = 0$ $W_{D} = \begin{cases} 3.40 + 0.37 \text{ E} (\text{E} \le 8 \text{ MeV}) \\ 6.36 \\ (\text{E} > 8 \text{ MeV}) \end{cases} r_{oD} = 1.26; a_{D} = 0.58$ $V_{so} = 6.20; r_{oso} = 1.12; a_{so} = 0.47$
(e) 93 <sub>Nb</sub> FOLDING POTENTIAL (9) (10)	$V_{R} = 54.51; r_{o} = 1.21; \mu_{R} = 2.10$ $W_{D} = 2.12; r_{oD} = 1.26; \mu_{D} = 1.57  (at E = 10 \text{ keV})$ $V_{so} = 6.72; r_{oso} = 1.12; \mu_{so} = 1.43$

# TABLE 1

(a) Standard O.M. parameters of Becchetti Greenlees; (b,c,d) O.M. parameters of Lagrange obtained from the SPRT method; (e) folding potential [46].
 V<sub>R</sub>, W<sub>D</sub>, W<sub>v</sub>, V<sub>so</sub> are in MeV; geometrical parameters are in fm.

target	89 <sub>Y</sub>	93 <sub>Nb</sub>	152 <sub>Sm</sub>	154 <sub>Sm</sub>	186 <sub>W</sub>	232 <sub>Th</sub>	238 <sub>U</sub>	238 <sub>U</sub>
nucleus								
s <sup>th</sup> o	0.47	0.43 0.41 (a)	1.79	1.28	2.31	1.00	0.94	0.95
s <sub>o</sub> exp	0.32±0.11	0.36±0.06	2.20±0.40	1.80±0.50	2.15±0.46	0.84±0.08	1.10±0.10	1.10±0.10
s <sub>1</sub> th	3.40	5.26 5.11 (a)	1.40	1.44	0.82	1.72	1.96	2.14
s <sub>1</sub> <sup>exp</sup>	4.40+2.00	5.16±0.24	-	-	0.76±0.30	1.60±0.20	1.70±0.30	1.70±0.30
R' <sup>th</sup>	6.78	6.63 6.97 (a)	8.02	7.65	7.18	9.45	9.08	9.24
R'exp	6.70±0.10	7.00±0.20	8.20±0.70	8.20±0.70	7.30±0.20	9.65±0.08	9.40±0.30	9.40±0.30
β2	0	0	0.22	0.24	0.213	0.206	0.216	0.216
β <sub>4</sub>	0	0	0	0	-0.060	0.086	0.067	0.067
Coupling	_	-	0 <sup>+</sup> -2 <sup>+</sup> -4 <sup>+</sup>	0 <sup>+</sup> -2 <sup>+</sup>	0 <sup>+</sup> -2 <sup>+</sup> -4 <sup>+</sup>			
Scheme	-	-	CFF	CFF	RFF	RFF	RFF	RFF

# TABLE 2

Calculations of s and p wave strength functions ( $S_0$  and  $S_1$ ) and potential scattering radii (R') for some nuclei. Comparison with experimental values taken from BNL-325, except for <sup>186</sup>W, whose measured  $S_0$  and  $S_1$  values are taken from CINDA (1974).  $S_0$  and  $S_1$  are in 10<sup>-4</sup> units and R' in tm. RFF = real form factor; CFF = complex form factor. (a) : results obtained from a folding potential (set (e) in Table 1).

1							,
r <sub>o</sub> = 1.17 Fm V <sub>R</sub> = 52.0 MeV adjustment to So, S1, R' (5)	1.05	2.07	9.23	15.70	11.73	8.00	6.48
$r_{O} = 1.17 Fm$ $V_{R} = 53.35 MeV$ $V_{R}r_{O}^{2} adjustment$ (4)	0.85	2.78	8.71	13.90	11.39	8,51	7.05
$r_{O} = 1.240 \text{ Fm}$ $V_{R} = 47.5 \text{ MeV}$ adopted parameters (3)	0.95	2.14	9.24	15.41	12.02	8.52	7.14
$r_{0} = 1.31 \text{ Fm}$ $v_{R} = 42.56 \text{ MeV}$ $v_{R}r_{0}^{2} \text{ adjustment}$ (2)	1.04	1.67	9.80	17.02	12,74	8.57	7.34
recommended values (1)	1.1 ± 0.1	1.7 ± 0.3	9.4 ± 0.3		12.21	8.62	7.18
	S <sub>o</sub> x 10 <sup>4</sup>	S1 x 10 <sup>4</sup>	R's fm	σ <sub>T</sub> (lOkeV) barns	σ <sub>T</sub> (100keV) barns	σ <sub>T</sub> (500keV) barns	σ <sub>T</sub> (1 MeV) barns

 $v_R r_o^n$  ambiguities for  $^{238}u$ 

TABLE 3

Recommended values for So, S1 and R' are taken from BNL 325, and total cross-sections from ENDF/BIV. See text for comments.

#### FIGURE CAPTIONS

FIG. 1: "s" wave elastic scattering phase-shifts (real part). The convergence is shown versus the number N of basis oscillator states, for different values of the oscillator parameter  $\beta$  (in fm<sup>-2</sup>). Calculations are shown at 2 MeV and 20 MeV for <sup>40</sup>Ca and <sup>238</sup>U. For both of them a spherical shape is assumed.

 $\mathbf{R}_{\max}$  (R<sub>n</sub>) is the matching (nuclear) radius. Results of numerical integration are also indicated (dashed lines). The potentials have the form (9) and (10), with the following values :  $V_{R} = 41.1 \text{ MeV}$ ;  $r_{0} = 1.374 \text{ fm}$ ;  $\mu_{R} = 1.5 \text{ fm}$  (see ref. [46]).

- FIG. 2: Optical model parameters (strength and geometry) versus :
  - 2a) mass number, as obtained from a study of 8 MeV neutron elastic scattering by HOLMQVIST and WIEDLING [49] (open circles : five parameters analysis ; solid circles : two parameters, V and W<sub>D</sub>, analysis)
  - 2b) neutron energy, as obtained by the same authors [50] from X<sup>2</sup> fits to measured elastic scattering cross sections of Cu.

### FIG. 3:

- 3a) Angular distributions for elastic and inelastic (first 2<sup>+</sup> state) scattering from <sup>186</sup>W for 3 MeV neutrons. Experimental data are from ref [70]. Compound elastic and inelastic contributions have been added to coupled channel calculations.
- 3b) Angular distributions for elastic scattering from <sup>148</sup> Sm and for elastic plus inelastic (first 2<sup>+</sup> state) from <sup>154</sup> Sm (squares), for 6.25 MeV neutrons. The solid lines through the data points are the results of coupled-channel calculations. The dashed line represents the calculated cross section for inelastic scattering (first 2<sup>+</sup> state) from <sup>154</sup> Sm [62].

FIG. 4: Total neutron cross section of <sup>238</sup>U. The curves are coupled-channel calculations using two sets of base states. The optical model parameters are that of Table 1, set (b), for (0<sup>+</sup>-2<sup>+</sup>-4<sup>+</sup>) coupling;
4a) 0.01 ≤ E ≤ 1.0 MeV Experimental data are from Ref. [100].
4b) 1.0 ≤ E ≤ 10.0 MeV Experimental data are from Ref. [101].

Total neutron scattering cross section of  $^{238}$ U. The curves are coupledchannel calculations using two sets of base states. The optical model parameters are that of Table 1, set (b), for  $(0^+-2^+-4^+)$  coupling; 4c) E = 4 MeV. Experimental data are from Ref. [102, 103, 104]. 4d) E = 7.54 MeV. Experimental data are from Ref. [105].

- FIG. 5: An example (given by TANAKA [57]) of the energy dependence of the optical potential depths. Open circles and crosses are the values obtained from parameter search using <sup>209</sup>Bi data [106] and <sup>207</sup>Pb [107] data respectively.
- FIG. 6: An example (given by BENZI [71]) of the effect of the optical potential parameters on calculated inelastic scattering of <sup>63</sup>Cu. Energy dependence of the potentials at energies higher than 3.5 MeV (full line) are shown in fig. A and B. Extrapolation of this energy dependence to low energies (see fig. A, B dashed line), and adopted energy dependence (see fig. A, B full line ) so as to obtain a good fit to inelastic scattering (see fig. C, D full line).
- FIG. 7: 7a) s-Wave strength functions for Tin, Tellurium and Xenon isotopes. Experimental values are taken from references [97,98,99]; dashed curves are calculations with the standard geometry of Perey, except for W. The optical potential includes a complex isospin term.
  - 7b) Elastic and inelastic differential scattering cross sections for  $^{76}$ Se and  $^{82}$ Se at an incident energy of 8 MeV. The dashed curves for elastic scattering are the results of a one channel, spherical potential fit to elastic scattering only. The solid curves are coupled channel calculations with  $\beta_2 = 0.27$  for  $^{76}$ Se and 0.19 for  $^{82}$ Se respectively. The dot-dash curve for  $^{82}$ Se shows the effects of a 10% increase in  $\beta_2$  on the inelastic scattering cross sections [85].

- FIG. 8: The measured total cross section difference divided by the <sup>148</sup>Sm total cross section for <sup>150,148</sup>Sm, <sup>152,148</sup>Sm and <sup>154, 148</sup>Sm. Also shown are coupled-channel calculations assuming rotational (full line) or vibrational (dashed line) models, for these nuclei. The various quadrupole deformation parameters were the following : 0.14, 0.17, 0.22, 0.24 for <sup>148</sup>, 150, 152, 154</sup>Sm respectively [86].
- FIG. 9: Excitation functions of the neutron inelastic scattering from the first excited state 2<sup>+</sup> of <sup>238</sup>U. The solid curves are : (ID) coupled-channel calculations using the LAGRANGE's <sup>238</sup>U potential [66], (CN) Hauser-Feshbach-Moldauer calculations using penetrabilities from the same deformed potential. The dashed and dot-dash curves are the results of Hauser-Feshbach-Moldauer calculations using penetrabilities from spherical potentials given, respectively, by KOLESOV [93] for <sup>238</sup>U, and by FU and PEREY [34] for Pb. The experimental values are taken from ref. [65].
- FIG.10: Compound nucleus formation cross section from the target <sup>238</sup>U calculated by using : (solid curves) the LAGRANGE's <sup>238</sup>U deformed potential [66]; (dashed, and dot-dash curves) the spherical potentials given, respectively, by KOLESOV [93] for <sup>238</sup>U, and by FU and PEREY [34] for Pb.
  - 10a) E < 0.8 MeV
  - 10b) 2 MeV < E < 20 MeV and comparison to experimental values extracted from the compilation [108].



FIG. 1





(a)

(ь)

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FIG. 2



FIG. 3 (a)

FIG. 3(b)

- 306 -





FIG.4

- 307 -







FIG.6

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FIG. 7\_(a)







FIG.9

7



(a)



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Review Paper No. 6

### PRE-EQUILIBRIUM EMISSION

### IN NEUTRON-INDUCED REACTIONS

Ъy

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## ABSTRACT:

In this paper the concept of the pre-equilibrium decay of compound systems in the framework of the Exciton Model is reviewed from the point of view of fast neutron-induced reactions. In the first part, a brief formulation of various modifications of the Exciton Model is given. In the second part a survey of the results obtained from the analysis of neutron-induced reactions shows, that the model allows one to reproduce quantitatively the main features of these processes, indicating that it is a powerful tool for neutron data evaluation work. Finally, some open questions of this concept are considered.

## I. INTRODUCTION

Pre-equilibrium emission of particles from highly excited states of compound systems seems to be now a well established fact. During the last years several models have been elaborated, which describe in a similar way this type of reactions [1-6]. Development of these models was stimulated by a large amount of experimental data that appears to deviate systematically from predictions of both extremely opposite nuclear reaction models used so far: direct reaction theory and statistical compound nucleus theory.

Moreover, there are physical arguments supporting the introduction of pre-compound models: If we classify nuclear reactions according to the time scale on which they occur, we can see, that direct reactions and compound nucleus processes define the two extremes of this time scale.

Direct processes involve a few degrees of freedom, which are excited in one or two collisions. Therefore, the emitted particle leaves the compound system in a time, which is in the order of the transition time for the projectile going through the nucleus. The momenta of projectile and emitted particles are strongly correlated, leading to a typical forward-peaked diffraction structure of angular distributions. Low-lying levels of residual nuclei are excited with high selectivity in respect to the wave functions of these states.

A quite different situation takes place once the long-lived compound nucleus state is reached. Depending upon excitation energy and single particle state density, a considerable part of all nucleons is excited and the energy and momentum of the emitted particle are independent of the way of formation of the compound nucleus. The decay probability is strongly predicted by the value of phase space which is accessible for the final systems, leading to the well-known Maxwellian spectrum of emitted particles. Assuming a continuous development of the compound system along the time scale, it is obvious to conclude, that between these two extreme reaction mechanisms intermediate processes should occur. The concept of pre-equilibrium decay consists in such a continuous development of a compound system via a series of successive interactions. The enormous difficulties connected with a correct quantuum mechanical time dependent treatment of nuclear reactions stimulated the development of several semiclassical approaches to this problem. At least three different approaches have been suggested:

- Geometric Intranuclear Cascade Monte-Carlo calculations;
- Fermigas Relaxation Model with the Master Equation system;
- Exciton Model, with some different modifications.

In this paper the present status of the Exciton Model and its applications to neutron-induced reactions in the energy region, which is relevant to the neutron data problem, is reviewed and some open questions of this model are considered briefly.

### 2. THE EXCITON MODEL

In 1966 Griffin [1] proposed a non-equilibrium statistical model for nuclear reactions based on the assumption that the interaction of the incoming particle with the target nucleus creates a simple initial configuration, which in the independent particle approximation can be characterized by a small number of excitons n (particles p plus holes h) and the excitation energy. Successive two-body residual interactions between particles and holes leads through a sequence of states with increasing exciton number to the compound nucleus state, e.g. to the statistical equilibrium. At each stage of this equilibration process there is a competition between the following decay modes of the compound system: Emission probability  $w_i$  for a particle of type i and transition probability  $\lambda_i$  to more or less complex intermediate states.

A brief review of the mathematical formulation of the Exciton Model and its different modifications is given in contributed paper 12 (reference [7]) to this meeting.

## 3. ANALYSIS OF FAST NEUTRON INDUCED REACTIONS

3.1 Inelastic scattering (n,n')

See contribution [7] to this meeting.

3.2 (n,p) reactions

Previous analysis showed, that the statistical theory of nuclear reactions did not allow a correct absolute description of both (n,p) cross-sections and proton spectra shape at 14 MeV incident energy, especially for heavy nuclei.

Total cross sections of a great number of elements with A>100 were studied by Braga-Marcazzan et al. [8]. They found a satisfactory agreement between pre-equilibrium calculations in the framework of Exciton Model (without any equilibrium component!) and experimental cross sections. The average value of transition probability  $\lambda_+$  (n = 3) was found in good agreement with those deduced from (n,n') spectra and (p,n) excitation functions (as mentioned in [7]). Excitation functions of (n,p) reactions were analysed with equilibrium and pre-equilibrium theory by Decowski et al. [9]. They have shown that the importance of taking into account pre-equilibrium mechanism is growing with excitation energy. Even for mediumweight nuclei pre-equilibrium emission at incident energies higher than 10 MeV is significant.

The proton emission spectra from heavy nuclei are almost completely reproduced by the pre-equilibrium model [8].

3.3 Reactions (n,2n) and (n,pn)

See contribution [10] to this meeting.

# 3.4 $(n, \alpha)$ reactions

As in the case of (n,p) reactions, the statistical model predictions of the 14 MeV induced  $(n,\alpha)$  cross sections on heavy nuclei are much smaller than experimental values.

Some special problems, however, are connected with the application of pre-equilibrium model to reactions with complex particles, such as  $\alpha$ -particles. The analysis of Milazzo-Colli et al. [11] and Glowacka et al. [12] show, that the exciton model allows one to reproduce satisfactorily the  $\alpha$ -particle spectra by the assumption, that  $\alpha$ -particles are preformed particles in the target nucleus, which are treated in a similar manner as the usual excited particles p. The absolute values of cross sections depend strongly on the introduced preformation probability  $\varphi$ , which was found between  $\varphi$ =0.8 and 0.1 for many nuclei with A >140 [11].

An other way is the many-particle approach to complex particle emission, which assumes, that  $\propto$ -particles are formed from excited quasi-independent nucleons (particles p) during the reaction, [13, 14]. This approach fits  $\propto$ -spectra worse in comparison with the previous method. But, as yet, definite conclusions supporting one of the two methods can not be drawn.

3.5 Application of Exciton Model to evaluation of neutroninduced reactions

See contribution [15] to this meeting.

### 4. OPEN QUESTIONS AND CONCLUSIONS

## 4.1 Angular distributions

The description of angular distributions represents at present one of the most important unresolved problems in the preequilibrium decay. An attempt on this problem recently has been performed by Ignatyuk et al. [16], who divides initial configurations of the compound system into open configurations (at least one particle unbound) and closed configurations. Further development of these configurations is assumed to be different: Open configurations lead to direct reactions, which are described by well developed models. Closed configurations are responsive for pre-equilibrium decay. Particles, emitted from these pre-equilibrium states Ignatyuk supposed to have a symmetric angular distribution:

$$\left(\frac{d\sigma}{ds}\right)^{\text{preeq}} \sim 1 + \frac{\overline{J}^2 \overline{\ell}^2}{12 \sigma_n^4} \cos^2 \vartheta$$

where

J - is the spin of compound system  $\ell(\varepsilon)$  - the orbital momentum

 $\sigma_n$  - an effective spin cut-off parameter for n exciton states ( $\sigma^2 > \sigma_n^2$ ).

This expression is analogous to the well-known semiclassical Ericson formula for angular distribution of particles emitted from compound nucleus. Analysis of <sup>56</sup>Fe(nn') at 14 MeV led to following conclusions: The sum of calculations by direct, pre-equilibrium and compound nucleus theory gives a good overall agreement of both the spectra and angular distributions of emitted neutrons. In the medium energy region of emitted particles the pre-equilibrium emission is essential, whereas the high-energy part is mostly due to direct processes.

Some other authors tried to explain the angular distribution of continuous spectra in the framework of direct reaction theories by averaging direct single particle or collective excitations over the energy. One kind of such a work is presented as a contributed paper to this meeting by Reif and Arndt [17]. In the framework of a microscopic approach to the scattering process, the high energy part of (nn') spectra at 14 MeV incident energy for  $40_{Ca}$  and  $56_{Fe}$  has been calculated with the well developed DWBA method. A good description of angular distribution is obtained also. Due to the microscopic consideration of all possible single-particle excitations this kind of calculations is rather difficult.

Similar results have been obtained with a collective model approach by Lewis [18]. More simple calculations on the base of plane wave approximation instead of distorted waves, and including simplifying assumptions on the formfactor have been reported by Lukyanov et al. [19] and similar results are presented by Jahn [20] as a contribution to this meeting. Altogether we can state the following: Exciton Model in the present form is based mainly on phase space considerations and energy conservation, but it does not imply any correlation between the momenta of incoming and outgoing particles.

And so, although it contends the direct one particle-one hole-excitation of residual nucleus as the first reaction step (pre-equilibrium emission from a 3-exciton state of compound system), Exciton Model describes only total emission spectra and absolute cross sections but not the angular distribution of emitted particles. One way to overcome this shortcoming is, to split partially (as done by Ignatyuk [16]) or totally the first interaction term from the pre-equilibrium reaction sequence and remove it by the result of calculation in the framework of a one-step theory of direct reactions. In this case it is possible to include also direct collective excitations of low-lying states, which is not included at all in the first term of the Exciton Model. Further investigations of this point are needed. As yet, different authors start from different definitions of what are direct and preequilibrium processes and usually the term "direct process" is identified with the result of calculations in the framework

of a direct reaction theory, leading to the erroneous conclusion, that pre-equilibrium processes are quite different from direct processes.

From physical point of view one of the most attractive feature of the Exciton Model is the following: The solution of the Master Equations taking into account all possible intranuclear transitions  $\Delta n = 0$ ,  $\pm 2$  yields both pre-equilibrium and equilibrium spectra and cross sections on a unique base. This advantage is lost if a part of pre-equilibrium emission is calculated by another theory - the direct reaction theory.

Therefore, attempts are made to include angular momentum in the Exciton Model. The first step in this direction was done by Blann [2] introducing the so-called Geometry Dependent Hybrid Model. However, this model is rather crude, especially for low and medium energy and, therefore, it was not applied successfully to the angular distribution problem.

Recently encouraging results on pre-equilibrium angular distributions, including angular dependence into the master equations, were reported by Weidenmüller and coworkers [21, 22].

Another attempt was made by Reif and Mädler [23] in the framework of non-equilibrium statistical formalism of Zubarev, including momentum conservation.

# 4.2 Conclusions

It was shown, that the concept of pre-equilibrium decay expressed in the Exciton Model formalism has a rather wide field of application in analysis of fast neutron-induced reactions. It is possible to calculate on an absolute base the overall magnitudes of cross sections and spectra shapes for a variety of nuclear reaction channels in a wide energy range without the aid of adjustable parameters (other than introduced by the optical model and statistical theory) in a simple statistical manner. Open questions beside the problem of angular distributions remain the mechanism of pre-equilibrium emission of complex particles. Pre-equilibrium emission of  $\gamma$ -rays is as yet not investigated at all. Only a few attempts have been made for investigation of the influence of structure effects (pairing and shell effects) on the pre-equilibrium decay.

As yet, this model has no theoretical foundation. Much further work is necessary to prove the Exciton Model with the formal theory of nuclear reactions, but there have been started some hopeful treatments in this direction [24, 25].
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Review Paper No. 7

#### FISSION THEORY AND ITS APPLICATION TO THE COMPILATION OF

NUCLEAR DATA

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#### Abstract

The paper describes the current status of fission theory with particular reference to its value in computing nuclear data (heavy element cross-sections, fission product yields, fission neutron emission yields etc.) for the purposes of nuclear power technology. The first major section reviews the calculation of deformation potential energy barriers from the best current theories and assesses the current accuracy of such calculations. Next, the theoretical determination of the potential energy surface between the saddle and scission points, governing the mass yield of fission products is reviewed. This is followed by the consideration of dynamical effects in the structure of crosssections and in the mass-yield problem. After this, statistical methods are reviewed. The principal conclusion of the paper is that current theory cannot produce reliable estimates of nuclear data from first principles, but it can give very important guidance on the systematic behaviour of important parameters that can be linked to experimental observations, and this allows quite reliable estimation of unmeasured data. Directions in which the theory can be improved in the near-future, with advantage to the nuclear data problem, are suggested.

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<sup>-1</sup>, while the differential fission cross-sections of fast neutrons of <sup>235</sup>U, <sup>239</sup>Pu and <sup>238</sup>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 measurement, while at the same time the range of nuclei for which sophisticated data are required is increasing rapidly. 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.

In these circumstances it is pertinent to ask to what extent can nuclear theory be used to alleviate the situation, and in this paper the particular case of fission theory is reviewed. There has been a tremendous surge of activity in the field of fission theory since the work of Strutinsky [1] and the discovery of the double-humped fission barrier in 1967. (Because of this the present review can be little more than an outline survey of the present status of fission theory). 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 scope of this paper therefore is to show how the theory connects and systematises a variety of experimental data, and thus reveals parametrisations which can be used reasonably reliably in quantitative calculations.

#### 2. Potential energy surfaces

The primary pre-occupation of fission theory has been the determination of the potential energy surface in the space of the various collective co-ordinates defining the shape of a deforming nucleus. Prior to about 1966 efforts in this direction concentrated on the liquid drop model. While this gave a qualitative account of the phenomenon of fission and simultaneously an overall semiquantitative description of nuclear binding energies it also had many difficulties (e.g. no obvious likelihood, in the light of the potential energy surface, of explaining asymmetric mass division, wrong trend of fission barrier heights). Myers and Swiatecki [2] first attempted to improve this situation by superposing shell effects in a semi-empirical way onto the liquid drop model, but it was Strutinsky [1] who made the real breakthrough in this direction by developing a more fundamental way of calculating the shell effects in such an approach, thus enabling the theory to be extrapolated to large deformations.

The basis of Strutinsky's method of calculating nuclear energies, either as a function of nuclear mass or as a function of deformation is now well-known. Very briefly outlined it is this: in a pure independent-particle shell model, particles (neutrons and protons) are filled into the levels of a deformed potential well (the deformation assumed static) up to a certain level (the Fermi energy) at which the particular nucleus of interest is obtained. The energies of the filled levels are then summed to give the nuclear ground state energy at the chosen well deformation. It is well-known of course that because of the residual interactions, and hence the correlated motions, among the nucleons, which cannot be described in the framework of a simple potential well model, this is a quite hopeless procedure for extracting the absolute energy of a real nucleus. For this the liquid drop model with semi-empirically adjusted parameters gives much more realistic estimates of the nuclear binding energies within 15 MeV or so at worst relative to binding energies of hundreds of MeV, over the whole periodic table; but it does not give any of the correlations with nuclear shell closures that appear in the observed binding energies.

Strutinsky's way of obtaining accurate estimates of absolute nuclear energies is to hypothesize that summing the single-particle state energies as shown in the left half of <u>Fig. 1</u> will reproduce the change in energy from nucleus to nucleus (at a given deformation) due to the shell structure, and to obtain this change, denoted by  $E_{\text{Shell Correction}}$ , it is only necessary to subtract from the independent-particle energy a similar sum calculated from the independent particle levels smeared out in some way to remove the shell structure, as illustrated schematically in the right half of <u>Fig. 1</u>. The gross energy that is thus removed is then replaced by a realistic energy term calculated from the liquid drop model  $E_{\text{LDM}}$ . Thus,

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$$E = E_{LDM} + E_{SC}$$
(1)

Strutinsky's method when applied to the broad mass of nuclei, with the energy minimised as a function of deformation for every nucleus, was immediately successful in reproducing accurately the nuclear binding energies. Furthermore, when the energy was calculated as a function of extended deformation for the actinide nuclei, in order to calculate fission barrier saddle heights to compare with observation, he discovered a secondary dip (Fig. 2) in the energy at deformations corresponding roughly to the traditional liquid drop saddle point. It is now well recognized that this deformation corresponds roughly to a spheroidal shape with a ratio of major to minor axes of about 2:1, and this gives almost as much shell structure (and hence great stability for particular nuclei like the actinides) as spherical potential wells (see Fig. 3 from ref. [3]). The dip or secondary well offered an explanation for the spontaneously fissioning isomers that had been known for a few years and for the phenomena of intermediate structure in fission cross-sections that were being discovered about that time, and Strutinsky's theory therefore became spectacularly successful.

Since Strutinsky's original work a tremendous amount of effort has been put into the calculation of potential energy surfaces as a function of deformation. Some of this has been devoted to discovering the possibility of new meta-stable shapes among the lighter nuclei, and much to the estimation of the stability of super-heavy nuclei with respect to alpha, beta and fission decay. As far as the subject matter of this paper is concerned, which is principally the fission properties, especially cross-sections, of the actinide nuclei, the theoretical work falls rather naturally into two divisions: the potential energy landscape in the region of the liquid drop saddle point, giving the double-humped barrier properties that control cross-sections; and the landscape beyond the barrier towards scission controlling in a more complex fashion phenomena such as mass division.

## 2.1 The Barrier Region

#### 2.1.1 Basis and technical treatment of Strutinsky theory

The justification of the Strutinsky method for determining nuclear energies, the technical method for carrying it out, and the physical nature of the results have been reviewed in detail by Brack et al [4]. A comprehensive review containing less detail but with a complete bibliography of work carried out up to 1972 has been written by Nix [3].

Basic justifications of the Strutinsky method start from the Hartree-Fock theory. In ref. [4] it is shown how the expression for the energy of a nucleus

in Hartree-Fock theory (in which the single-particle potential is selfconsistent with the single-particle density matrix generated by that potential) can be written in terms of shell-model single particle energies and densities to second order in the difference between the shell-model and the self-consistent densities. The significant feature of the new expression for the Hartree-Fock energy is that apart from the simple sum over occupied shell-model levels the remaining principal term is expressed in terms of <u>averaged</u> single-particle densities, and is therefore smooth in its dependence on nucleon numbers and nuclear shape. It is this smooth term plus a smooth component extracted from the sum over occupied single particle levels that is replaced by a liquid drop expression for the energy,  $E_{LDM}$ .

Most of the methods for extracting the smooth component from the sum of occupied energy levels are based on Strutinsky's own technical procedures for averaging over the shell-model energy levels with a suitable weighting function (see refs. [1,4]). This weighting function can be expressed as sums of products of Gaussians and Hermite polynomials, the width of the gaussian being governed mainly by the energy spacing between major shells just below the Fermi energy. Such averaging procedures can run into conceptual if not practical difficulties however if the shell-model potential is a realistic one i.e. it permits unbound eigenstates, as with the Woods-Saxon potential for instance. Bengtsson [5] has therefore initiated a method in which each individual shell-model level as a function of deformation is smoothed by fitting it with the cube root of a fourth-order polynomial in the deformation parameter; this particular form of the fitting function is suggested by the Thomas-Fermi statistical model. The smooth component of the sum of occupied energy levels is then simply given by the sum of the occupied smoothed energy levels resulting from this fitting procedure, and the unbound levels thus require no consideration. The shell correction energy,  $E_{SC}$ , thus defined for neutrons in <sup>238</sup>Pu is shown in Fig. 4 in comparison with the result from the same set of shell-model levels using the Strutinsky procedure. The overall agreement, especially for prolate deformations in which we are most interested in fission theory, is seen to be remarkably good, although local differences of up to 1 MeV can occur.

#### 2.1.2 Comparison with Hartree-Fock calculations

Apart from work on the justification of the Strutinsky theory in a basic way, there have been attempts to calculate nuclear deformation energies directly from Hartree-Fock theory. These employ the Skyrme effective nucleonnucleon interaction [6] with parameters adjusted to reproduce gross nuclear properties, as given in ref. [7]. The result of the work of Flocard et al [21] showing the binding energy for  $^{240}$ Pu as a function of the quadrupole moment of the nucleon density is presented in <u>Fig. 5</u>. No allowance is made for axial asymmetry or reflection asymmetry in the nuclear shape in this calculation. It looks qualitatively very similar to the deformation energy curves that result from calculations using the Strutinsky method but the energy differences between the extrema are greater. For example the first barrier height  $(V_A)$  is at about 9 MeV relative to the primary well depth  $(V_I)$  whereas Strutinsky calculations with a similar restriction on the range of nuclear shapes explored would give about 6 MeV for this quantity. However, there are recognized sources of error in the present Hartree-Fock calculation that approach the order of one MeV; they arise from the necessity to project out the 0<sup>+</sup> ground state from the calculated state with no constraint on angular momentum, and from the truncation of the harmonic oscillator basis states used in the numerical work.

# 2.1.3 Nuclear Models employed in Strutinsky calculations

Apart from the possible source of error arising from the actual principle of the Strutinsky theory, and possible errors from the technical treatment of smoothing procedures, the basic parametrisations of the models used in the theory contain uncertainties that will give rise to errors in calculations based on the theory. The main source of this kind of error is likely to come from the liquid drop model, which provides the basic (or macroscopic) energy term in the Strutinsky theory, but there are also likely to be significant uncertainties from the shell model adopted, and smaller errors from the treatment of the pairing interaction, which is shell dependent and is also normally incorporated into the Strutinsky theory. This last term depends not only on the choice of shell model but also on the hypothesis assumed for the dependence of the interaction strength on surface area. Notice, in this connection, that virtually all calculations with the Strutinsky method have been made for even nuclei.

# 2.1.3.1 Liquid Drop and Droplet Models

The nuclear energy in the basic liquid drop model of the nucleus is characterised by a volume term proportional to the mass number A, a surface energy term proportional to the surface area, and hence to  $A^{2/3}$  for a spherical nucleus, and a Coulomb energy term, proportional to  $A^{-1/3}$  for a spherical nucleus:

$$E_{LD} = -C_{v}A + C_{s}A^{2/3}B_{s}(shape) + \frac{3}{5}\frac{e^{2}Z^{2}}{r_{o}A^{1/3}}B_{c}(shape)$$
(2)

where  $B_s$  (shape) is the ratio of the surface area of the deformed nucleus of specified shape to that of a spherical nucleus, and  $B_c$  (shape) is the ratio of

the Coulomb energy of the deformed nucleus to that of the sphere. The quantities e and r<sub>o</sub> are the proton charge and the nuclear radius constant of proportionality, respectively. The coefficients  $C_v$  and  $C_s$  contain a dependence on the neutron-proton asymmetry I = (N - Z)/A:

$$C_v = a_v (1 - k_v I^2)$$
 (2a)

$$C_{g} = a_{g} (1 - k_{g} I^{2})$$
 (2b)

So far as the fission barrier is concerned, the important terms in equation (2) are the surface energy and Coulomb energy terms, and the sum of their contributions to the liquid drop energy relative to the energy of a spherical liquid drop can be written as

$$E_{LD}$$
 (shape) -  $E_{LD}(0) = \left\{ B_{s} (shape) - 1 \right\} + 2\pi \left\{ B_{c} (shape) - 1 \right\} E_{s}(0)$  (3)

where  $E_s(0)$ , the surface energy of a spherical liquid drop, is  $C_s A^{2/3}$  and **x** the fissility parameter is defined as the ratio of the Coulomb energy of a spherical drop to  $2E_s(0)$ :

$$\mathbf{x} = \left(\frac{3}{5} \left(\frac{e^2}{r_0}\right), \frac{(z^2/A)}{2a_s(1-k_s I^2)}\right)$$
(4)

The fissility parameter, and hence the values of the coefficients a and k, are crucial in determining the shape dependence of the liquid drop energy and therefore of fission barriers. These coefficients have to be determined empirically from an overall fit to nuclear binding energies and, where possible, to experimental fission barrier data. For reliable determination of the coefficients equation (2) is too crude as it stands, and it is recognized that in that formula the volume and surface terms are only the leading terms of a systematic expansion of the nuclear energy of a finite body with a relatively thin surface region in which the matter density falls to zero. The ratio of surface diffuseness to nuclear radius is of order  $A^{-1/3}$ , so a refinement of equation (2) takes the expansion to higher powers in  $A^{-1/3}$ ; this is the droplet model of Myers and Swiatecki [8]. In this, terms in  $A^{1/3}$  are associated with energy of curvature of the surface and redistribution of Coulomb energy in the surface, and other terms are associated with the compressibility of nuclear matter. The many parameters involved are determined partly from fitting to experimental data and partly from statistical calculations based on Thomas-Fermi theory; fitting to experimental data has to take account of shell effects both in ground-state masses and in fission barriers, and this is generally done in the empirical way outlined in ref. [2]. Values of the

liquid drop (or droplet) coefficients actually used for calculations of fission barriers by the Strutinsky method vary. One common set is that due to Myers and Swiatecki [9] (liquid drop model):

$$r_{o} = 1.2249 \text{ fm},$$
  
giving  $\left(\frac{3}{5}\right)\left(\frac{e^{2}}{r_{o}}\right) = 0.7053 \text{ MeV},$   
 $a_{s} = 17.9439 \text{ MeV}$   
 $k_{s} = 1.7826$  (5)

Another set coming into vogue is derived from a redetermination of droplet model coefficients in unpublished work of Myers and Swiatecki referred to in ref. [10]; from these an equivalent set of liquid drop coefficients can be determined, among which an effective neutron-proton asymmetry coefficient,  $k_{s,eff}$ , turns out to have the value 2.8. This implies a distinct lowering of the calculated values of the fission barriers of neutron-rich nuclei from those that would be calculated with the set (5), and at present it can be stated that the precise value of the surface neutron-proton asymmetry coefficient is probably the main uncertainty arising from the liquid drop or the droplet model in calculating fission barrier heights.

#### 2.1.3.2 Shell Models

There is wide variety in the choice of shell model for calculating the shell-correction energy entering fission barrier calculations. Strutinsky's own calculations [1], [5] employed a deformed Woods-Saxon potential which has the advantage of physical realism for nuclear shapes that are not too strongly deformed; the potential is defined in such a way as to have a constant skin thickness about an effective surface defining the shape. Such a potential encounters difficulties for strongly necked-in shapes, and here a variation suggested by physical notions of the effect of finite range nucleon forces has advantages; this is the diffuse-surface potential obtained by folding a Yukawa function over a square-well potential of the nuclear shape required [11]:

$$V(\vec{r}) = -\frac{V_{o}}{4\pi a^{3}} \int_{t}^{d} r' \frac{\exp[-|\vec{r} - \vec{r}'|/a]}{|\vec{r} - \vec{r}'|/a}$$
(6)

where  $V_0$  is the square well depth. The range, a, of the Yukawa function can be chosen to give the desired surface diffuseness. Parameters of such potentials are generally chosen to reproduce a given set of experimental data on single particle levels. Nix and his collaborators chose to fit their potential to the level of <sup>208</sup>Pb in their earlier calculations [11], but in a later set they have adjusted their parameters to fit the levels of heavy deformed actinide nuclei [12]. The difference in the two sets of potential well parameters amounts to about 11% in the surface diffuseness parameter (smaller in ref. [12]) and 12% and 6% in the neutron and proton spin-orbit interaction (greater in ref. [12]).

The other class of shell model potentials in common use is based on the harmonic oscillator. In general these have distinct computational advantages and permit the exploration of a greater variety of nuclear shapes. Calculations of the potential energy landscape in the region of the barrier are generally performed within the framework of the one-centre modified oscillator model with the shell model potential having, typically, the following form:

$$V = V_{osc} + V_{corr}$$
(7)

$$\mathbf{V}_{\text{osc}} = \frac{1}{2} \, \frac{\pi \omega}{2} \, \mathbf{\rho}^2 \left[ 1 - \frac{2}{3} \, \varepsilon \sqrt{\frac{4\pi}{5}} \, \cos \, \mathbf{Y} \cdot \mathbf{Y}_{20} + 2\varepsilon \, _4 \mathbf{P}_4 + \frac{2}{3} \, \varepsilon \sqrt{\frac{4\pi}{5}} \, \frac{\sin \, \mathbf{Y}}{\sqrt{2}} \, (\mathbf{Y}_{22} + \mathbf{Y}_{2-2}) \right]$$
(7a)

$$V_{\text{corr}} = -k \cdot \tilde{n} \overset{\circ}{\otimes}_{0} \left[ 2 \vec{l}_{t} \cdot \vec{s} + \mu \left( \vec{l}_{t}^{2} - \langle \vec{l}_{t}^{2} \rangle \right) \right]$$
(7b)

The correction term, depending principally on the square of the orbital angular momentum  $\hat{\ell}_t$ , has the effect of flattening the potential towards its outer edges and also contains a spin-orbit interaction. The parameters k and  $\mu$  are adjustable for optimal reproduction of experimental single particle level schemes. The variable **p** is the radius vector length in "stretched" co-ordinates and is thus defined by

$$\boldsymbol{\rho}^{2} = \frac{M}{n} \left( \omega_{\mathbf{x}} \, \mathbf{x}^{2} + \omega_{\mathbf{y}} \, \mathbf{y}^{2} + \omega_{\mathbf{z}} \, \mathbf{z}^{2} \right) \tag{8}$$

The oscillator frequencies for the principal ellipsoidal axes are related to the parameter  $\omega_0$  (itself governed by the shape parameters  $\epsilon$ ,  $\epsilon_4$  and  $\gamma$ ) through the relations

$$\omega_{\mathbf{x}} = \omega_{\mathbf{0}} \left[ 1 - \frac{2}{2} \varepsilon \cdot \cos\left(Y + \frac{2\pi}{3}\right) \right]$$
$$\omega_{\mathbf{y}} = \omega_{\mathbf{0}} \left[ 1 - \frac{2}{2} \varepsilon \cdot \cos\left(Y - \frac{2\pi}{3}\right) \right]$$
$$\omega_{\mathbf{z}} = \omega_{\mathbf{0}} \left[ 1 - \frac{2}{2} \varepsilon \cdot \cos\left(Y - \frac{2\pi}{3}\right) \right],$$

and  $\omega_0$  is related to the spherical oscillator frequency  $\omega_0^0$  through a volume conservation condition. A typical numerical value adopted for the last parameter is [13]

$$\mathbf{\hat{x}} \stackrel{0}{\underset{\mathbf{w}}{\overset{\mathbf{w}}$$

the plus and minus signs referring to proton and neutron potentials respectively.

The deformation parameters  $\xi$ ,  $\xi_4$  and  $\gamma$  refer to quadrupole deformation (nuclear elongation), hexadecapole deformation (waist-line "necking-in" or broadening) and degree of axial asymmetry, respectively. The parameter  $\gamma$  is generally treated through its range of values 0° to 60°, 0° representing axial symmetry of a prolate body and 60° the opposite extreme of axial symmetry of an oblate body. Other degrees of freedom in the shape can be introduced within this framework, still allowing practical computation, and two such important parameters are the deformations associated with the third and fifth Legendre polynomials; these parameters allow the description of reflection asymmetry in the nuclear shape (often referred to as mass or volume asymmetry).

More sophisticated shell-model effects can be incorporated within the Strutinsky theory. One of these is a shell-correction term to the Coulomb energy [14] which is normally computed simply as a liquid drop term with uniform charge density over the nucleus. For this, the Coulomb repulsion energy is calculated directly from the single particle wave-functions; the proton densities arising from these can change sharply with changing deformation giving rise to changes in the occupation of single particle levels near the Fermi energy with very different radial and angular distributions. The treatment of pairing correlation energies can also contain elaborations. One of these is the dependence of the pairing interaction strength on surface area, as already mentioned. Another is the introduction of the quadrupole pairing force [14]. This arises from the well-known expansion of a delta-force in terms of spherical harmonics,

$$\delta(\vec{r}_{1} - \vec{r}_{2}) = \sum_{\lambda \mu} \frac{\delta(r_{1} - r_{2})}{r_{1} r_{2}} \Psi_{\lambda \mu}(1) \Psi_{\lambda \mu}(2)$$
(10)

only terms in  $\lambda = 0,2$ ,  $\mu = 0$  being retained.

# 2.1.4 <u>Results of Calculations</u>

## 2.1.4.1 Inner Barrier

The shell correction as a function of deformation is obviously correlated with the local density of single particle levels in the shell model around the highest occupied level (in the absence of pairing correlations), the Fermi energy. High single particle densities give rise to a positive shell correction (less stability) and vice versa. An oscillating shell correction (with the correct phase) superimposed on or close to the liquid drop saddle point gives rise to the double-humped barrier. Variation of the shellcorrection amplitude or phase with changing proton and neutron number, together with the variation of the liquid drop potential barrier with changing fissility parameter, gives rise to variation of the double-humped barrier from nucleus to nucleus. The contribution to the shell correction from the pairing correlation effect is opposite in sign, being negative at high single particle densities, but is much smaller in magnitude than the main shell effect.

The phrase "double-humped barrier" expresses the main feature of the potential energy of deformation of the nucleus as a function of elongation of the nucleus towards fission. Early calculations assumed a maximum degree of symmetry in the shape in the course of this elongation. Pashkevich [15] first investigated the potential energy as a function of axial asymmetry along this path and noted that the secondary well in the barrier was stable with respect to this. Later work [16,17,18] has concentrated on investigating the potential energy surface in the plane of elongation and the Y-degree of freedom more carefully, and has established in general that the nucleus has axial asymmetry at the first saddle point (A) but has regained axial symmetry at the secondary well (II). Typical results of Larsson and Leander from ref. [18] are shown in Fig. 6. For  $^{236}$ Th the inner barrier occurs at a value of  $\Upsilon \approx 10^{\circ}$  but the potential energy on the axially symmetric path is only ~0.4 MeV higher than the saddle; whereas for  $^{250}$ Cm the barrier energy drop at an axial asymmetry Y  $\approx 17^{\circ}$ is a substantial 1.8 MeV. There is a trend for increasing stability of axially asymmetric shape at the inner barrier both with increasing neutron number and increasing mass number as shown in Fig. 7 (from ref. [18]). As far as the actual magnitudes of the barrier heights are concerned, the axially asymmetric values of Fig. 7 tend to be a little lower in general (on average ~0.5 MeV) than experimental data (after making allowance for zero-point /3 -vibration energy of the ground state). For the Th nuclei they are considerably lower, but there may be special reasons in theory and interpretation of experimental data for this. For each element the trend of the calculated value with neutron number is gently peaked at N  $\approx$  150. The experimental data (see Fig. 31 Section 5) show similar trends but with the peaking 2 to 3 neutron units lower.

The agreement of this kind of calculation with data seems to be improved if the quadrupole pairing interaction is included [14], particularly for Th nuclei for which the inner barrier is raised by about 1 MeV. For Pu nuclei

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quadrupole pairing raises the inner barrier by about 0.5 MeV. It should be noted that in the calculation of Larsson et al [14] the liquid drop energy has been refitted so that the calculation reproduces experimental data on the secondary well.

#### 2.1.4.2 Secondary Well

Calculations on the energy of the second minimum relative to that of the first minimum, this time due to Möller and Nix [12] (using still the modified harmonic oscillator shell-model potential), are shown in <u>Fig. 8.</u> In general these energies are in the range 2 to 3 MeV and agree with available experimental data on spontaneously fissioning isomers to this extent. However, interpretation of experimental fission cross-section data on Th isotopes (see for example ref. [37]) indicates that the secondary well is higher than 4 MeV for these light nuclei and so disagrees with the trends of the calculation.

The overall trend of the curves in <u>Fig. 8</u> (with a minimum about N  $\approx$  145 and a peak about N  $\approx$  152) is also given by calculations using the folded Yukawa model [12]. However, there are discrepancies in absolute value of up to ~0.5 MeV between the two sets of calculations, changing in sign between Th and Fm.

#### 2.1.4.3 Outer Barrier

Early calculations in which the nuclear shape was assumed axially and reflection symmetric indicated that the outer barrier was higher than the inner one in the actinides by some 3 to 4 MeV (see <u>Fig. 2</u>). Experimental data on spontaneous fission isomer half-lives and excitation cross-sections and intermediate structure in fission cross-sections refuted this; indeed analysis of data on plutonium and higher nuclei suggested that experimentally the outer barrier is the lower. The discrepancy was removed at least qualitatively by the calculations of Möller and Nilsson [19,20] demonstrating that reflection asymmetry in the nuclear shape (included in the shell-model potential as thirdand fifth-order Legendre polynomials) gave potential energy minima at the elongations corresponding to the outer barrier. There is no calculational evidence for axial asymmetry also existing at the outer barrier. Indeed, the existence and explanation of strong angular distributions of fission products is held to be evidence against axial asymmetry.

More recent calculated values of the outer barrier height [12] are shown in <u>Fig. 9.</u> The curves for individual elements do not show marked structure or trends (except for the highest elements) but there is a strongly falling tendency with increasing nuclear charge, which is borne out by experimental data on fission isomer excitation yields. These calculations employ a modified harmonic-oscillator shell model potential, and they show discrepancies of up to ~1 MeV (changing sign in going from Th to Fm) with calculations based on a folded Yukawa potential (eq. 6).

The calculations based on the folded Yukawa shell-model potential [12] show a new feature in the potential energy curve in the second barrier region; this is a tendency in the low Z, moderate N nuclei for the outer barrier to be further split into two subsidiary peaks with a shallow minimum between them (see <u>Fig. 10</u>). If this is a real physical effect it will explain experimental fission data on Th isotopes which demand an interpretation involving a double barrier peak with a very shallow well between them.

# 2.1.4.4 Probable Accuracy of Quantitative Calculations on Fission Barrier Parameters

In <u>Table 1</u> the theoretical results on fission barriers for two specific nuclei are compared. These are both nuclei that are quite central to the nuclear stability line and to the actinide group of elements and therefore ought to provide reasonable tests for theoretical calculation. Some of the differences in the numbers are of course due to very significant differences in the physics assumed, e.g. degree of asymmetry in shape allowed, but even where sets of numbers are comparable, because differences are confined to the choice of shell-model, as in rows 1 and 3 (columns 3 to 5) or rows 1 and 2 (column 6) differences of the order of 1 MeV in the estimated quantity occur. This can probably be taken as a measure of the accuracy of the theory at the present time. This statement is supported by a comparison of the measured nuclear ground state masses of the actinides and lower nuclei with the values calculated by Möller and Nix [12] using the folded Yukawa shell-model within the Strutinsky theory; the average discrepancy is about zero, but there are systematic trends of the discrepancy curves as a function of neutron number, the trends having a slope of  $\sim 0.5$  MeV per neutron. The accuracy of the theory is extremely good when set against the nuclear binding energies of well over 1000 MeV, but they are not accurate to supply on their own the relevant barrier parameters for the nuclear cross-sections required by technology.

## 2.2 Potential Energy Between Saddle and Scission

The point to emerge from the theoretical calculations of the kind described in Section 2.1.4.3, that the saddle point at the outer barrier of the bulk of actinide nuclei occurs for reflection asymmetric nuclear shapes, invites the speculation that this is the reason for mass asymmetry in the final mass division of these nuclei. Much further work has been done on this point, and forms one of the most interesting later developments based on Strutinsky's original work, leading towards an apparent solution of the formerly intractable problem of mass asymmetry in fission. In broad terms, the theoretical work has concentrated on mapping-out the energy surface well beyond the outer saddle point and well down the slope towards the scission point where the two incipient fission fragments finally part company. By contrast with the region of deformation up to the outer saddle point, this region is a hazy ill-understood area from the overall point of view including the dynamical effects; the whole question of nuclear viscosity arises here in a very important way. There is a general feeling that viscosity must act selectively. Some quantities seem to be frozen in at the saddle point e.g. the projection of the nuclear spin on the major axis of deformation, thus determining the angular distributions of the fission fragments relative to some laboratory-based axis that is significant in the original formation of the excited fissioning nucleus. The finding of mass-asymmetry in the energy surface at the outer barrier at first sight indicates that the broad trends of mass division in the final fission products may also be largely frozen in here.

This point of view is now disputed by much more recent calculations by Mustafa et al [22] using the two-centre shell-model [23,24]. This is another elaboration of the Strutinsky method, with the novel feature that the shell model potential is composed of two deformed harmonic oscillator wells with a variable distance between their centres that represents the major fission parameter, the elongation. This scheme is particularly appropriate for a description of the later stages of fission when the two wells describe the individual nascent fission product, although there can be some difficulties of treatment in the neck region. Mustafa et al do achieve a satisfactory smooth neck join, and one their four independent deformation parameters is the neck radius, D, others being the volume ratio of the incipient fragments, and two co-ordinates describing elongation of the fragments.

The folded Yukawa shell-model treatment [12] (see eq. 6) is also very well-suited for treatment of the potential energy of deformation between saddle and scission, no ambiguities arising in the treatment of the neck region.

The broad picture is indicated by <u>figures 11 to 17</u>. <u>Fig. 11</u> is the energy surface for <sup>210</sup>Po as calculated by Mustafa et al [22]. The ordinate in this diagram is the radius of the neck between the incipient fragments; decreasing neck radius is correlated with increasing elongation of the fissioning system. The abscissa is the degree of reflection asymmetry relative to the neck, interpreted here in terms of incipient fragment mass. The diagram shows that the primary well, intermediate barrier and secondary well all have reflection or mass symmetry although the secondary well is already becoming very broad in this respect. The dominant outer barrier however gives definite energy favouring to a very considerable degree of mass asymmetry, but this is rapidly lost with increasing elongation. Energetically, for above-barrier fission mass asymmetry would still be allowed at the scission point if the conditions at the outer barrier controlled the mass division, but, experimentally, symmetric mass division is found for this nucleus.

<u>Fig. 12</u> is a similar diagram for  $^{236}$ U also calculated by ref. [22]. In this case the degree of mass asymmetry at the outer barrier is largely but not quite conserved at the scission point. The experimental situation of course is that the fission of  $^{236}$ U is very asymmetric at low or modest energies, but the peak to valley ratio corresponds to a neck radius on this diagram where the minimum energies are several MeV below the saddle point energy.

Fig. 13 gives the same kind of information, but in a sketchier way, for  $^{252}$ Fm. Here the energy behaviour is given as a function of volume ratio (or mass division - top scale) for cuts through the potential energy surface at a number of fixed values of neck radius. The top curve corresponds to the outer fission barrier, and here it is apparent that mass symmetry is favoured. By the time the scission point is approached, however, a considerable minimum has been developed at a volume ratio of 1.25. The same tendency, although less marked, is found for <sup>256</sup>Fm, calculated by the same methods in ref. [25]: see Fig. 14. In <sup>200</sup>Fm, by contrast, mass asymmetry never becomes favoured in the energy diagram (Fig. 15) although the minimum becomes increasingly shallow towards scission. The experimental evidence on Fermium fission generally favours the idea that the mass distribution is largely controlled by the energy surface near scission. Data by Raigaini et al [26] on thermal neutron-induced fission of <sup>255</sup>Fm and <sup>257</sup>Fm are shown in <u>Fig. 16</u> indicating an increasing trend to symmetric fission at <sup>258</sup>Fm, while spontaneous fission of <sup>250</sup>Fm as measured by Flynn et al [27] shows the characteristic doublepeaked mass asymmetric curve with a peak to valley ratio of 12:1. However the mass yield is very sensitive to energy availability and its division among degrees of freedom. This is shown already for <sup>256</sup>Fm by the difference between its spontaneous fission and its fission following formation by adding a slow neutron to  $^{255}$ Fm. The correlation, in the latter case, between mass yield and the total kinetic energy of the fission fragments is also suggestive [26]; this is shown in Fig. 17. It would appear that the fragments with high kinetic energy are very much more sensitive to the potential energy contour at low neck radius (as shown in Fig. 14) than are those with low kinetic energy.

The overall conclusion from studies of this kind is that the mass yields in fission are determined, to the extent that the potential energy surface contributes a crucial role in mass division, by the potential energy characteristics several MeV below the outer saddle point, rather than at the saddle point itself. This alone points to the fact that the dynamics of the problem must be of vital importance in controlling the mass division; and the difficulties of drawing conclusions from potential energy calculations alone are emphasized by <u>Fig. 18</u> which is to be compared with <u>Figs. 12 and 15</u>. The potential energy surfaces of <u>Fig. 18</u> (calculations from ref. [12]) are in the plane of deformation variables one of which (distance between mass centres) is defined in a different manner from that of <u>Figs. 12 and 15</u> (neck radius). The valleys leading toward mass asymmetry for <sup>235</sup>U and towards mass symmetry in  $^{258}$ Fm are much less well defined in <u>Fig. 18</u>. Part of the difference must certainly be due to the difference in basic physical models, but part will also certainly be due to the necessity of knowing the relevant inertial tensors in order to define the most likely trajectories of the physical system through these landscapes.

## 3. Dynamical Considerations

The potential energy landscapes for deformation of the nucleus discussed in Section 2 provide the essential foundation for discussing the fission process and suggest already many of the most striking phenomena to be observed, but, with such complicated potential energy surfaces, and with the consideration that the nucleus is a microscopic body, strongly influenced by the motion of a single or a few nucleons, it is apparent that the dynamics of fission is still a major problem. The difficulties are compounded in two main ways. Firstly, for large deformations from a spherical shape, a description of the deformation in normal modes, based on a Legendre polynomial expansion of the surface, is not practicable; the choice of suitable deformation parameters is somewhat arbitrary, although based on physical intuition, and as a result the inertial tensor can take a complicated non-diagonal form. Furthermore, the inertial tensor is strongly affected by single particle effects as well as being a measure of "collective motion". Secondly, the effects of "viscosity" in the nuclear motion obviously play an important role. Viscosity is itself a classical concept and its transference to the nuclear case is not yet clearly defined, although there is much current work on this topic (see e.g. ref. [28]). Many of the quantities observable in fission (e.g. cross-sections at low energies, properties of spontaneously fissioning isomers) do not require such an all-embracing concept as viscosity for their explanations; these can be based on extensions of normal quantal ideas. On the other hand, some fission phenomena involve such a large number of degrees of freedom that statistical or thermodynamic treatments seem to be demanded.

#### 3.1 Inertial Tensor Calculations

The dynamical requirement of an expression for the kinetic energy in terms of generalised collective co-ordinates  $q_i$ ,

$$\mathbf{T} = \frac{1}{2} \sum_{i,j} B_{ij}(\mathbf{q}) \, \dot{\mathbf{q}}_{i} \, \dot{\mathbf{q}}_{j}$$
(11)

demands the knowledge of the inertial tensor as a function of the collective co-ordinates. This is the essential complement to the potential energy and can be either modelled according to hydrodynamic concepts [29] or can be computed microscopically from the same shell model level schemes used to construct the shell-correction to the potential energy in the Strutinsky method. The classical liquid drop model is already sufficiently complex that straightforward analytical expressions for the inertia have not been derived except for very small deviations from a sphere, in which case the inertial parameter associated with the lowest normal mode (the quadrupole term in the spherical harmonic expansion of the surface) for irrotational flow is

$$B_{/3} = 3M R_0^2 / 8 \pi$$
, (12)

/3 being the coefficient for the second spherical harmonic  $Y_{20}$  in the expansion of the surface, M the nuclear mass and  $R_0$  the nuclear radius. For his studies of the later stages of fission towards the scission point Nix [30] used the Werner-Wheeler numerical method, in which the internal hydrodynamic flow is approximated by the flow of circular layers of fluid perpendicular to the symmetry axis.

Phenomenological expressions for the inertia have also been employed; for example if the fragment separation r is employed as the fission variable the asymptotic inertial parameter at large separations, r is the reduced mass of the fragments,  $\mu$ , while at the other extreme of small deformation it tends toward eq. (12) for irrotational flow. A typical expression for  $B_{rr}$ , due to Randrup, quoted by Szymanski [31], is

$$B_{rr} = \left\{ 1 + \frac{17}{15} k \exp \left[ - (r - 0.75 R_0)/d \right] \right\} \mu.$$
(13)

where  $R_0$  is the spherical nuclear radius, and k and d are parameters that describe deviations from the irrotational value (for irrotational flow k = 1, d =  $R_0/(2.542)$ .

Microscopic calculations of the inertial tensor are normally based on the cranking model, originally developed by Inglis [35] for calculation of nuclear

moments of inertia, in which the independent particle or quasi-particle system is assumed to be driven in a specific form of collective motion by an external force, and the inertial parameter is determined from the generated kinetic energy and the collective velocity. Its application to fission was first developed by Sobiczewski et al [32] and Damgaard et al [34]. The cranking model expression involves virtual excitations from the ground state | o> of the deforming system to excited states | m>:

$$B_{ij} = 2 n^{2} \sum_{m \neq 0} \frac{\langle 0 | \partial / \partial q_{i} | m \rangle \langle m | \partial / \partial q_{j} | o \rangle}{E_{m} - E_{0}}$$
(14)

For a pure independent particle system this expression, literally evaluated, contains singularities at single-particle level crossings. Within the shell-correction framework of the Strutinsky theory, however, pairing forces are included in the shell-model treatment; the resulting energy gap separating the ground-state from other states removes these singularities and permits the inertial tensor to have a behaviour of reasonable physical magnitude. A simple statistical expression for the dependence of the inertia on the energy gap,  $\Delta$ , and the density of single particle states,  $g_{eff}$ , at the Fermi energy is developed in ref. [34]:

$$B \sim \frac{\hbar^2}{2} \left| \frac{\partial H}{\partial q} \right|^2 \frac{g_{eff}}{\Delta^2}$$
(15)

A typical detailed calculation of the inertia from the cranking model is shown in <u>Fig. 19</u>; this is due to Pauli and Ledergeber [36]. As to be expected from eq. (15) it is strongly correlated with the shell-correction to the potential energy of deformation of the nucleus. This strong structure in the inertial parameter already implies that the potential energy alone does not provide a simple guide to the dynamical motion of the system through deformation space.

This is demonstrated by Pauli and Ledergeber's treatment of spontaneous fission half-lives. The half-life is proportional to the Gramow barrier tunnelling factor

$$U \sim \frac{1}{\omega} \exp\left[-2 \frac{s}{\hbar}\right]$$
  
$$S = \int_{q_1}^{\sqrt{q_2}} dq \sqrt{2B_q \left[E - V(q)\right]}$$
(16)

The integral S, the action integral, is calculated along a trajectory q through deformation space, defined to give the least value of S. The inertial parameter

 $\boldsymbol{B}_{_{\boldsymbol{Q}}}$  for this trajectory is determined from the inertial tensor by

$$B_{q} = \sum_{i,j} B_{ij} \frac{\partial q_{i}}{\partial q} \frac{\partial q_{j}}{\partial q}$$
(17)

The trajectory calculated from this prescription for symmetric deformations in  $^{240}$ Pu is shown in Fig. 20. It is apparent that the "dynamic" barrier for this trajectory is higher than the static barrier. Calculations of spontaneous fission half-lives of ground states using these calculations of the inertia and the least action principle give remarkably close agreement with data provided that the surface energy constant of the liquid drop model is suitably adjusted (see Fig. 21). This, as shown in the diagram, differs for different elements. Agreement is poorer (discrepancy up to four orders of magnitudes) if it is attempted to use a universal surface energy constant. Half-lives of spontaneously fissioning isomers are shown in Fig. 22.

Pauli and Ledergeber suggest as a hypothesis that the least action trajectory determined for spontaneous fission should also be the path for near-barrier fission. While this would have the attraction of explaining the high intermediate barriers observed for Th isotopes (the dynamic barriers found for these are particularly high compared to the static barriers [44]), it is certainly a very controversial idea and needs to be properly tested by a calculation of the development of the wave-function over the barrier in a two- or few-dimensional deformation space.

# 3.2 Structure of Shape Isomers and Related States

## 3.2.1 Single Particle States

The properties of the spontaneously fissioning isomers associated with the secondary well of the double-humped barrier can be discussed by means of fairly standard nuclear dynamical methods and models. The single particle character of low-lying states associated with the secondary well can be obtained by extensions of Nilsson diagrams to the greater deformations, as already calculated for the purpose of forming the nuclear potential deformation energy in the Strutinsky theory. A typical single particle diagram for the extended deformation at the second minimum is shown in <u>Fig. 23;</u> this has been compiled by Vandenbosch [42] from computations of various authors. Data on highly deformed single particle levels that can be tested against the predictions of such diagrams are already available. For example, in <sup>231</sup>Th it is known that  $I^{\pi} = 1/2^{-}$  and  $3/2^{-}$  neutron levels occur close to the Fermi energy [37], and in <sup>237</sup>Pu the two lowest single particle levels at the secondary well deformation lie within a few hundred keV, and have probable spin values of I ~ 5/2 (for the lowest, 0.1  $\mu$  s state) and I ~ <sup>11</sup>/2 (for the 1.1 $\mu$ s state) [39,40]. The g-factor of the magnetic moment of the latter has been measured [41], and has been interpreted as indicating that the orbital angular momentum and spin of the odd neutron are anti-parallel in this state, thus giving information about the possible Nilsson orbital. The <sup>231</sup>Th states could be explained by the [510]<sup>1</sup>/2<sup>-</sup> and [512]<sup>3</sup>/2<sup>-</sup> orbitals embracing the 140 neutron Fermi level in two of the level schemes of <u>Fig. 23</u>, but there seem to be no levels close to the Fermi surface having the properties necessary to explain the sophisticated observations made on the <sup>237</sup>Pu isomers.

## 3.2.2 Rotational Bands

The deformed shell model level schemes can also be used to determine the moment of inertia of the rotational bands associated with the spontaneously fissioning isomers. Generally, the cranking model of Inglis [35] is used for these calculations, and the pairing force is included. A typical calculation on  $^{240}$ Pu, which is very similar in result to a similar calculation of Sobiczewski et al [43] is shown in <u>Fig. 24</u>. Specht et al [78] have made direct observations of the electromagnetic transitions between the rotational states in the isomer band, from which the moment of inertia has been determined to be very close to the calculated value. The effective moment of inertia of the secondary well state of  $^{251}$ Th has also been determined from measurements of fission product angular distributions [37]. Because this is an odd-particle nucleus and the effective moment of inertia can be distorted by Coriolis coupling, its value is less directly comparable with theory, but semi-quantitatively it shows the effect indicated in <u>Fig. 24</u>, that its value is about twice that expected for a ground state rotational band.

## 3.3 Intermediate Structure in Cross-sections

Cross-sections for fission reactions that proceed at energies close to or below fission barriers show structure that is amenable to quantum-mechanical treatment and, often, to theoretical nuclear structure considerations. General discussions of such treatments were given originally by Lynn [45] and Weigmann [46]. The basic feature of them is that basis states can be classified as belonging to the region of deformation space close to either the primary well (class-I states) or the secondary well (class-II states). The interaction between these sets of states that gives rise to the intermediate structure can be described by the matrix elements of an interaction term in the Hamiltonian of the system:

$$H^{int}_{\lambda_{I}\lambda_{II}} \equiv \langle \lambda_{I} | H^{int} | \lambda_{II} \rangle$$
(18)

This interaction can be expected qualitatively to be similar to the terms that

already give rise to the complexity of compound nucleus states at moderately high excitation energies. However, because of the very small overlap in deformation space between the class-I and class-II states implied by the existence of the intermediate barrier between the primary and secondary wells, the matrix elements in (18) are very small, the actual value being mainly governed by the height of the intermediate barrier relative to the excitation energy.

The physical nature of the class-I states is known experimentally from the properties of neutron resonances and, to a lesser extent, from studies of stripping reactions, and can be extrapolated to higher or lower energies. These properties are typically reduced neutron widths, which give the probability of excitation by neutron bombardment or (d,p) reactions, radiative widths, giving the probability of radiative decay, and level density. The class-II states are inferred to have zero reduced neutron width, a total radiative width of value a little different from that of the class-I states (and a different radiation spectrum), and a density certainly much less than that of the class-I states at the same energy. They will also have an appreciable fission decay width. The class-II state density will depend on the excitation energy available after subtraction of the potential energy of deformation at the secondary well, and the fission width  $\Gamma_{\lambda_{II}}(F)$  will depend on the relative height of the outer barrier.

The exercise of coupling a single class-II state to a large number of class-I states in the same energy region using the matrix elements (18), gives the coefficients of admixture of the class-II state into the actual virtual levels of the compound nucleus system. The fission widths of these levels are approximated by the Lorentzian expression

$$\overline{\overline{\Gamma}}_{\lambda(F)} = \frac{D_{\lambda}}{2\pi} \frac{\Gamma_{\lambda II(c)} \Gamma_{\lambda II(F)}}{(E_{\lambda II} - E_{\lambda})^2 + \frac{1}{4} (\Gamma_{\lambda II(c)} + \Gamma_{\lambda II(F)})^2}, \quad (19)$$

(with the bar expressing a local energy average to suppress the individual fluctuations of Porter-Thomas character that are expected), provided that the class-II "width",  $\Gamma_{\lambda II(c)} + \Gamma_{\lambda II(F)}$ , is appreciably greater than the fine-structure level spacing  $D_{\lambda}$ ; otherwise equation (19) has to be stated more precisely [45]. The class-II coupling "width"  $\Gamma_{\lambda II(c)}$  appearing in this expression is related to the matrix elements through

$$\Gamma_{\lambda_{II(c)}} = \frac{2\pi H^{Int 2}}{D_{\lambda_{I}}}$$
(20)

Normally, in the energy region of application of equation (19) the class-I states are of complicated character. The class-II states on the other hand may be of comparatively simple structure, particularly if the secondary well is shallow. This seems to be the case in the Th isotopes, and is demonstrated by the neutron-induced fission cross-section of <sup>230</sup>Th (fig. 25). The single peak in the cross-section shows strong and changing patterns of angular distribution of fission products, and these data have been interpreted as a superposition of Lorentzian patterns of fission widths, as in eq. (19), one for each rotational member of a band based on a class-II state with the simple structure of an odd-neutron with  $\Omega^{\pi} = 1/2^{-1}$  coupled to a beta-vibration in the secondary well [37]. The number of phonons in the beta-vibration is not known but is expected to be low (probably not more than one), otherwise it would be expected that this simple state would become at least partially mixed with class-II states of more complicated character (such as three quasi-particle states) and the fission cross-section would appear correspondingly complicated. The analysis of the <sup>250</sup>Th data also gives magnitudes for the intermediate and outer barrier height.

Certainly in higher-charge nuclei the class-II states appearing at the excitation energies induced by slow neutrons are much more complicated, as shown in <u>Fig. 26</u> (the fission cross-section of  $^{237}$ Np as measured by Michaudon [47]). In this, the first and most dramatic example of narrow intermediate structure observed in neutron-induced fission cross-sections, the class-II state spacing is only ~50 eV (c.f. the class-I spacing is ~0.7 eV), implying that about  $3\frac{1}{2}$  MeV of excitation energy is available to these states and that the secondary well is only about 2 MeV higher than the primary well. The widths and strengths of the intermediate structures can again be interpreted to give semi-quantitative information on the heights and tunnelling characteristics of the intermediate and outer barriers.

# 3.4 Dynamical Treatment of Mass Yields

The differences in mass yield behaviour due to energy availability and its division as shown in the fission of  $^{258}$ Fm <u>(Fig. 17)</u> recall the essential point of having to include the dynamics of the system in the treatment of the mass yield problem. The calculations of the potential energy surface described in Section 2 give no more than the possibility of being able to calculate the correct quantitative mass yield curves. A start has been made on the dynamical problem by work like that of Maruhn et al [48] in which the volume asymmetry  $\lambda$ is treated as a dynamical collective co-ordinate and the corresponding inertial parameter is calculated from the quasi-particle levels of a shell-model with pairing force, using the cranking formula (eq. 14). With knowledge of the

inertial parameter and the potential energy the Schrödinger equation for the wave-function in the volume asymmetry co-ordinate can be solved. In principle a two-dimensional (at least) Schrödinger equation, including the elongation variable, E , is set up but it was established in practice that the inertial was much smaller than the square root of  $\sqrt{B_{\lambda\lambda}}$   $B_{\epsilon\epsilon}$  so matrix element B that it could be assumed that there was very little dynamical coupling between the two collective variables. In a completely adiabatic model of spontaneous fission of the ground state only the lowest energy state among the solutions of the Schrödinger equation is required; this gives (by squaring) the mass-yield curve. The results of such calculations confirm that to get the peaks of the mass yield curves at the correct mass numbers the potential energy surface at least several MeV below the saddle point is the controlling factor (see Fig. 27 for spontaneous fission of  $^{236}$ U); this is in spite of the fact that the inertial parameter also includes sharp fluctuations. In addition, however, it turns out that in the adiabatic model the mass yield peaks are too sharp. Maruhn and Greiner [49] then consider a superposition of excited state wave functions in the volume asymmetry co-ordinate, weighting these according to a Boltzmann factor. The temperatures required in this Boltzmann factor to obtain agreement with experimental data are of the order of 0.5 - 2 MeV. With this model Maruhn and Greiner also obtain qualitative agreement for fission of Ra (triple-peaked mass yields) and neutron-induced fission of <sup>257</sup>Fm (symmetric fission with elevated wings; see Fig. 16).

# 4. Statistical and Thermodynamic Methods

The necessity, in the work of Maruhn and Greiner [49] described in Section 3.4, of introducing a temperature concept for the superposition of mass asymmetric wave functions, in order to reconcile theory and experiment (even though dynamic coupling between the mass asymmetric mode and the elongation mode appeared negligible), leads to the general discussion of statistical and thermodynamic methods in fission theory. The two can best be differentiated by describing statistical methods as those that construct excited state densities from shell-model level schemes to give the phase space volume over a range of values of the deformation, the available excitation energy being deduced from the deformation energy surface constructed for zero excitation of the nucleus, while thermodynamic methods are those that assume an excitation of the nucleus to a specific temperature and calculate the excited deformation energy surface at that temperature. The application of the two kinds of methods to various phenomena will be discussed in parallel in the sections below.

## 4.1 Mass Yields, Fission Energy Distribution and Related Quantities

In modern statistical calculations of mass yields the potential energy surface V(q) (for zero excitation) as determined by the Strutinsky method is used as the basis for calculating available excitation energy  $E^*$  from the total energy at a specific deformation q

$$\mathbf{E}^* = \mathbf{E} - \mathbf{V}(\mathbf{q}) \tag{21}$$

This is then used to determine the density of states of internal excitation at the deformation q,  $\rho$  (q,E\*), from which in turn the probability of the nucleus occupying that deformation is determined [50]:

$$P(q) dq \approx \Theta^{n_q/2} \rho(q, E^*) dq \qquad (22)$$

where

$$\Theta = \left(\frac{\partial \ln \rho}{\partial E'}\right) E' = E^*$$

and  $n_q$  is the number of collective degrees of freedom involved in the nuclear motion.

In the work of Jensen and Damgaard [51] and Jensen and Døssing [52] the deformation variables q considered are specified as elongation c, neck radius h and volume asymmetry  $\lambda$  . Calculations of the probability P(q) are made as a function of volume asymmetry,  $\lambda$  , at specified points c, h in the valley between outer saddle and scission. The potential energy surface is calculated from the Woods-Saxon shell model of [4] and liquid drop parameters of [36]. The level density  $\rho$  (E\*) is calculated from the single-particle scheme of the chosen shell model by standard numerical methods (see e.g. [53]), including pairing correlations, to give the density of independent quasi-particle states with angular momentum projection K on the cylindrical symmetry axis of the nucleus; the density of states with total angular momentum I is determined by summation from K = -I to I. For reconciliation of data and calculation over a wide range of energy it appears that the elongation cannot be too large ( $c \leq 1.65$  x spherical nucleus diameter, which is not much below the outer saddle); for this elongation a comparison of data on the position of the heavy fragment peak, the peak width and the peak to valley ratio for <sup>240</sup>Pu are given in Fig. 28. For <sup>258</sup>Fm, however, agreement is not found between experiment and theory up to elongations of c = 1.70; it is believed that this is due to inadequacy of the shell model in this transitional region.

Calculations of a similar kind have been carried out by Kapoor and Ramamurthy [55] using  $^{242}$ Pu as an example. For elongations corresponding to the second barrier, the mass distribution, if determined at that point, is

highly asymmetric at low compound nucleus excitation energies, and changes to symmetry at about 20 MeV. The peak widths at low excitations are much too small, however, and this indicates again that the mass asymmetry is determined several MeV below the outer saddle point.

In thermodynamic calculations as exemplified by the work of Schmitt and Mustafa [56] it is assumed that internal excitation of the nucleus to a temperature  $\Theta$  gives rise to a probability distribution for the occupation of single particle levels of the Fermi type

$$p_n = \left\{ 1 + \exp[(\varepsilon_n - \varepsilon_F) / \Theta] \right\}^{-1}$$
(23)

for single particle levels of energy  $\varepsilon_n$ . From this the sum of single particle excitation energies  $\varepsilon_0 = 2\sum \varepsilon_n p_n$  is calculated for a specific nucleon number  $N = 2\sum \varepsilon_n p_n$ , from which the Fermi energy  $\varepsilon_F$  is deduced. A smoothly varying total single particle energy can also be defined

$$\widetilde{E}_{\Theta} = 2 \int_{-\infty}^{\infty} d\varepsilon \sum_{n=1}^{\infty} \frac{\varepsilon \widetilde{g} (\varepsilon, \varepsilon_n)}{1 + \exp[(\varepsilon - \widetilde{\varepsilon}_F)/\Theta]}$$
(24)

the Fermi energy  $\tilde{\epsilon}_F$  of the smoothed distribution of levels  $\tilde{g}(\epsilon, \epsilon_n)$ , being deduced from the particle number

$$N = 2 \int_{-\infty}^{\infty} d\varepsilon \int_{n=1}^{\infty} \frac{\widetilde{g}(\varepsilon, \varepsilon_n)}{1 + \exp[(\varepsilon - \widetilde{\epsilon}_F)/\Theta]}$$
(25)

The shell-correction energy for temperature 0 is

$$\mathbf{E}_{SC} = \mathbf{E}_{\Theta} - \widetilde{\mathbf{E}}_{\Theta}$$
(26)

(there are actually two of these terms, one each for neutrons and protons) and this, added to the liquid drop energy, eq. (3), gives the deformation energy  $E_{DEF}$  at this temperature. At the same time the internal excitation energy  $E^*$  is given by

$$\mathbf{E}^* = \mathbf{E}_{\Theta} - \mathbf{E}_{\Theta=\Theta} \tag{27}$$

Typical calculations of the deformation energy have been carried out in this way for  $^{236}$ U. They show that the shell-correction energies for different neck sizes (taken as a measure of elongation of the fissioning system) and different volume asymmetries,  $\lambda$ , approach zero with increasing temperature, the major variation occuring between  $\theta = 1$  to 3 MeV. The deformation energy itself as a function of volume ratio for different values of neck radius and temperature is shown in Fig. 29. These show the transition from mass asymmetry to symmetry, as given by the minimum in the deformation energy to take place at a temperature of  $\theta = 1.8$  MeV, corresponding to an internal excitation energy of about 90 MeV.

The above thermodynamic calculations have been made using an extension of the Strutinsky method for deformation energies, and this approach has been checked by Brack and Quentin [57] using a Hartree-Fock self-consistent method. Essential agreement is found although there is some compression of the upper part of the shell model spectrum at higher temperatures and the smooth part of the Hartree-Fock energy (the "liquid-drop" term) shows some temperature dependence.

Statistical theories for fission mass yields of the kind outlined in this section are, of course, a modern variant of much older work along these lines; work of the kind initiated by Fong [58] rested on the hypotheses that the mass yield was governed by the level density of the system at the scission point as a function of mass asymmetry, and that the available excitation energy was governed by the shell structure of the incipient fragments. The last factor was parametrised whereas in the modern work it is calculated within the Strutinsky theory. However, the modern work is still phenomenological to the extent that the fundamental question of exchange of energy between collective modes and intrinsic (single particle) excitation is avoided. In the statistical theories it is assumed that all available energy above the minimum required deformation energy becomes intrinsic excitation energy up to a specific elongation, which is determined by fitting the data; beyond this elongation the implicit assumption is made that the mass distribution is frozen, presumably by further elongation to the scission point being "sudden". In the thermodynamic theories no assumption is made about exchange of energy; intrinsic excitation is related to a temperature  $\theta$ , and it would be hoped that both this parameter (and hence the actual sharing of energy between collective and intrinsic mode) and the elongation at which the mass division becomes frozen would be revealed by fitting the theory to mass yield data as a function of excitation energy.

Thus, the chief role that the statistical and thermodynamic theories play at present is to provide a tool for analysis of experimental data in a way that allows further understanding of the role of nuclear viscosity between the fission barrier and the scission point. It follows that until this understanding emerges no fundamental theory of the ultimate energy division in fission, and hence of total neutron yields,  $\overline{\nu}$ , energy spectra of the emitted neutrons and gamma-ray yields from the fission products, is possible. These quantities, which together give the total excitation energy of the separated fission products, do not immediately give the intrinsic excitation energy prior to scission; to this must be added the deformation energy of the incipient fission fragments and coulomb excitation energy in the early stages just following scission. Full account of these factors suggests that probably no more than half the potential energy difference between saddle and scission is converted into intrinsic excitation energy [60].

Phenomenological theories of such quantities as neutron yield exist (see e.g. the work of Sarkar and Chatterjee [59] and references therein), which by use of statistical nuclear level density models can reproduce such observations as the saw-tooth variation of  $\overline{\nu}$  with fission product mass number.

Other more controversial observations, such as the variation of  $\bar{\nu}$  with the initial compound nucleus excitation energy at low energies (some experimenters claim that there is a change of slope of  $\bar{\nu}$  against incident neutron energy below about 1 MeV; for a brief review and references on this topic see [61]), are equally controversial in explanation. Such a change of slope in  $\bar{\nu}$  could be explained by the preservation of superfluidity between saddle and scission for an even-even nuclear system crossing the barrier in the lowest transition state, which is fully pair-correlated; this view is supported by observations of mass-yield fine structure favouring even-even fission products (experimental data of Unik et al [62] and Nifenecker et al [63]; for a review of the situation see Bjørnholm [65]). It is also supported by theoretical considerations of Nörenberg [64] who finds that in a level-crossing model coupling between collective states is strong whereas that between intrinsic nucleonic excitations is weak.

## 4.2 Fission Cross-sections

The compound nucleus formation cross-section for neutron energy  $E_n$  (to which corresponds a de Broglie wave-length, divided by  $2 \gamma$ ,  $\lambda_n$ ) is given in terms of the transmission coefficient  $T_{J(n)}$  (for total angular momentum J):

$$\sigma_{n,CN}(E_n) = \pi \chi_n^2 \sum_{g} g_J T_{J(n)}$$
(28)

where  $g_J$  is the statistical spin weighting factor. Simple Hauser-Feshbach theory [66] for compound nucleus reactions can be used to determine a partial reaction cross-section into a channel c from this formation cross-section:

$$\sigma_{nc} = \pi \lambda^2 \sum_{J} \frac{T_{J(n)} T_{J(c)}}{\sum_{c'} T_{J(c')}}$$
(29)

These cross-section expressions are for averages over any local resonance fine

structure that may be present. If the neutron energy is so low (or the angular momentum so high) that narrow resonances do exist the transmission coefficient can be written in terms of the average resonance partial width  $\bar{\Gamma}_{(c)}$  and spacing  $\bar{D}$ :

$$T_{(c)} = \frac{2\pi \Gamma(c)}{\overline{D}}$$
(30)

At high neutron energies when  $\overline{\Gamma} \gg \overline{D}$ , the transmission coefficient approaches unity.

Statistical nuclear reaction theory is very familiar for particle reactions. A summary of its application to neutron reactions, especially neutron inelastic scattering and radiative capture can be found in ref. [67]. Here we are concerned with its application to fission. The fission transmission coefficient (through a single Bohr channel, f [70]) is based on the original statistical theory employed by Bohr and Wheeler [68], together with an estimate of the quantal tunnelling through a harmonic potential barrier [69]:

$$T_{(f)} = \left\{ 1 + \exp\left[-2\pi (E - E_{f})/\hbar \omega_{f}\right] \right\}^{-1}$$
(31)

Here,  $E_f$  is the peak height of the harmonic barrier (including the intrinsic excitation of the Bohr channel), and the tunnelling characteristic  $\pi \omega_f$  is related to the curvature of the potential barrier about  $E_f$  and the inertial parameter associated with the collective motion through the barrier. For a single-humped barrier of this kind, the total fission transmission coefficient  $T_{(F)}$  is the sum of the individual  $T_{(f)}$  over all Bohr channels f. The density of these is denoted by the density of states of excitation in all intrinsic degrees of freedom at the barrier deformation,  $\rho^{(F)}(U)$ . Thus

$$\mathbf{F}_{J(F)}(E) = \int_{0}^{\infty} dU \, \rho^{(F)}(U,J) \frac{1}{1 + \exp\left[-\frac{2\pi(E-V_{F}-U)}{\hbar\omega_{F}}\right]}$$
(32)

where  $V_F$  is the peak barrier deformation energy, and  $\hbar \omega_F$  is assumed equal, for all fission channels, to a common value  $\hbar \omega_F$  for the barrier concerned.

The double-humped nature of the fission barrier of the actinides, which results from Strutinsky's theory of deformation energies and is supported by a wealth of experimental evidence, introduces important modifications into the formulation of the fission transmission coefficient. If equation (32) is defined separately for the two barriers (inner, A and outer, B, as illustrated in <u>Fig. 1</u>), a statistical theory of the decay rate across the double barrier (making due allowance for the compound system formed in the secondary minimum after transmission across barrier A then returning across barrier A) [71,72,73] gives an effective fission transmission coefficient

$$T_{(eff,F)} = \frac{T(A) T(B)}{T(A) + T(B)}$$
(33)

provided that one or both of  $T_{(A)}$ ,  $T_{(B)}$  is of the order of unity or greater.

Where both the transmission coefficients  $T_{(A)}$ ,  $T_{(B)}$  are considerably less than unity, eq. (33) becomes inadequate for obtaining the fission cross-section by substitution in the Hauser-Feshbach formula, eq. (29). This is because the fission cross-section then exhibits narrow intermediate class-II structure (or perhaps gross vibrational structure) as described in Section 3.3. Fission competition with other reactions is then localised into the regions of the class-II resonances, and the simple proportionality  $T_{(eff,F)}/\sum_{c'} T_{(c'')}$ is no longer an adequate expression of the average fission probability,  $\bar{P}_{F}$ . An expression for the fission probability derived in a uniform picket-fence model of the resonance structure is [74]

$$\overline{P}_{F} = \left[1 + \left(\frac{\sum_{c} u^{T}(c^{u})}{T_{(eff,F)}}\right)^{2} + 2\left(\frac{\sum_{c} u^{T}(c^{u})}{T_{(eff,F)}}\right) \operatorname{coth} \left(\frac{1}{2} T_{(A)} + \frac{1}{2} T_{(B)}\right)\right]^{-1/2}$$
(34)

where the sum labelled by c" refers to all channels other than fission.

With barrier heights determined (within, say, the framework of Strutinsky theory) the key to the calculation of fission cross-sections at higher energies lies in the evaluation of the density of intrinsic excitations at the fission barriers,  $\rho^{(A)}(U)$ ,  $\rho^{(B)}(U)$ , occuring in eq. (32). As in statistical theories of the mass yield these densities can be determined from the positions of the single particle levels around the Fermi energy at the deformation in question. Programmes on these lines have been carried out by Britt et al [53] and Metag et al [75]. Although the single particle level densities are greater at the saddle points (at least for symmetric deformation) than at the primary and secondary minima and intuitively therefore it would be expected that the independent many-particle states built up from them would be greater in density at a given excitation, the surprising result is obtained (see Fig. 30) that the barrier densities are slightly lower than the well densities up to excitation energies of several MeV; this is because of the role of the pairing force, which considerably increases the magnitude of the energy gap separating the lowest state from the two or more quasi-particle states for the high single particle state densities at the saddle deformations. These calculated intrinsic state

level densities, when inserted into the expressions for fission cross-sections with realistic barrier heights, result in calculated cross-sections that are considerably lower than experimental values.

This has led to the realization of the important role played by collective rotations in the level structure and the correspondingly important influence of the symmetry of the nuclear shape [76]. Calculations of level density based on the independent-particle model give rise to the density of intrinsic states,  $ho_{_{
m BH}},$  which act as heads to rotational bands, and cannot be expected to include the rotational members of these bands and other collective excitations at least up to moderate excitation energies. If only the rotational states (being the most numerous collective states) are considered, it is apparent that the enhancements to the calculated intrinsic state density can be large. For a nucleus with axial and reflection symmetry, each intrinsic state with spin projection K along the cylindrical symmetry axis carries a rotational band with spin member I = K, K + 1, K + 2, ... (except for K=0 for which I = 0, 2, 4, ...). For values of spin I that are small compared with  $290/h^2$ , where 3 is the moment of inertia about an axis perpendicular to the cylindrical symmetry axis and  $\Theta$ is the temperature parameter of the level density, these rotational states augment the density of the band-head states by a factor of the order of  $\frac{90}{\hbar^2}$ ; for low to moderate excitation energies and normal deformations of actinide nuclei this is expected to have a numerical value of the order of 25 to 40.

Such shape symmetry and the corresponding rotational level enhancement factor is expected to be applicable to the calculation of the total transmission coefficients for inelastic neutron scattering,  $T_{(n)}$  and radiative capture  $T_{(\gamma)}$ . The theory of potential energy surfaces indicates that the fission saddle points do not possess a similar degree of symmetry. The outer saddle point, B, is believed to be reflection asymmetric. This introduces an extra rotational band of states for each intrinsic state possessing opposite parity (for K=O, the extra rotational members have  $I = 1, 3, 5, \dots$ , giving rise to an extra factor of 2 in the rotational enhancement factor of the level density. The inner saddle point A possesses reflection symmetry but normally does not have axial symmetry. According to Bjørnholm, Bohr and Mottelson [76] this gives a collective enhancement factor of the order of  $[(\pi/2) \prod_k (\frac{4}{5} k^{0/\pi^2})]^{\frac{1}{2}}$  (where the  $d_k$  are the moments of inertia about the three principal axes of the nucleus) over the intrinsic level density; numerically this implies an enhancement factor of the order of 5 to 10 with respect to cylindrically symmetric shapes. These numerical factors will appear in the barrier transmission coefficients, and give a corresponding enhancement to the calculated fission cross-sections. For a shape with no rotational symmetry another factor of 4 enhancement in the rotational level density occurs.

Gavron et al [77] have incorporated such rotational enhancement factors corresponding to reflection asymmetry for barrier B and complete asymmetry for barrier A into computations of the independent quasi-particle state densities and have achieved reasonable numerical agreement with the fission probability observed for many ( ${}^{3}$ He,dF) and ( ${}^{3}$ He,tF) reactions on actinide nuclei.

# 5. Application of Fission Theory to Cross-section Data and Related Quantities

From the review of the previous sections it is apparent that fission theory has not yet achieved the quantitative status that would allow it to be used for the reasonably accurate computation of technologically required nuclear data starting from fundamentals. The theoretical determination of fission barriers, the first requirement, is not accurate to better than between 0.5 to 1 MeV, whereas technology demands an accuracy of the order of 100 keV. Inertial tensor parameters have only been computed for spontaneous fission, with considerable apparent success, but it is by no means clear that the same methods would do for excited state fission. Ideas on the potential energy landscape towards the scission point on inertia and on viscosity are sufficiently well developed to make it seem very likely that a qualitative understanding of fission product mass-yields has been achieved, and that an understanding of energy division and neutron emission will follow but reliable quantitative predictions are nowhere likely to be achieved on a short time-scale.

Nevertheless fission theory has an important role to play in the nuclear data field. There is sufficiently detailed qualitative and semi-quantitative understanding for a wide range of phenomena to be reconciled. It is this kind of understanding which is invaluable in providing a framework for the systematics of interpolating and extrapolating parameters used in calculations of nuclear data.

The cross-sections of the actinides are an example of this. A recent systematic attempt [67] to reconcile all available data relating to fission cross-sections and other cross-sections affected by fission competition is based on obtaining the barrier level densities by adjustment, within the framework of the double-humped barrier model, to a few well-measured cross-sections  $(^{246}Cm, ^{238}U, ^{232}Th, ^{237}Np, ^{241}Am, ^{235}U, ^{239}Pu)$  up to neutron energies of a few MeV. These barrier level densities, assumed to form a six-part set (for barriers A and B and for even, odd-A and odd nuclei) universal to the actinides, are related in turn to the level density parametrization chosen for normal deformations; the latter are designed to reproduce observed neutron resonance spacings, inelastic neutron spectra, radiative capture gamma-ray spectra and neutron energy variation of neutron capture cross-sections.

The barrier level densities so found are, at barrier A, a factor of 4 to 5 higher than the normal level density at the same equivalent excitation energy,

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and the barrier B density is a factor of ~2 higher (although this is less certain because the evidence rests to a considerable extent on the cross-sections of Th and Pa nuclei which show a great deal of vibrational resonance structure rather than smooth quasi-plateaux in their energy variation). These factors are almost certainly the rotational band enhancement factors discussed in Section 4.2. These, together with a determination of barrier heights that follow much of the trends discussed in Section 2.1.4, are vital in explaining the wide variation in magnitude of fission cross-sections from Th to Cm for a variation in <u>effective</u> barrier height of less than 1 MeV.

The deduction of barrier level densities in this way already implies a knowledge of fission barrier parameters. For the nuclei employed in the survey of ref. [67] the barrier parameters were determined by detailed fitting of neutron-induced fission cross-sections and other data (e.g. (t,pF), (d,pF),  $({}^{3}\text{He},dF)$  fission probabilities [85]) below and up to the barrier energies. For the even nuclei studied in this fitting procedure, physically reasonable models of the low-lying discrete channel structure across the barriers were adopted, and for all nuclei the detailed effect of coupling of class-I and class-II states, resulting in the expression (34) for the fission probability, was taken into account. This coupling is particularly important for the analysis of fission probability data on even compound nuclei, for which the fission barriers generally lie below the neutron separation energy. In these cases the weak radiative capture competition is greatly enhanced by the concentration of the fission into narrow intermediate resonances, and this can cause an effective "raising" of the fission barrier by up to 0.5 MeV.

The final results on barrier parameters cannot be taken as unique because of the number of parameters involved (at least 4:  $V_A$ ,  $\hbar\omega_A$ ,  $V_B$ ,  $\hbar\omega_B$ ). The penetrability parameters in general were fixed to the values determined in the best fits to the key cross-sections listed above. The outer barrier height,  $V_{p}$ , is generally the least well-determined parameter. It appears to be about the same value as the inner barrier for U and Np nuclei and a little higher than  ${\rm V}_{\rm A}$ for Th and Pa. A semi-quantitative indication of its value in Pu, Am and Cm nuclei, in which it becomes decreasingly important, has been determined from analysis of excitation curves for the formation of spontaneously fissioning isomers [73, 53], and this was used as a guide in the work of [67]. The inner barrier heights, relative to the ground state, are shown in Fig. 31. Like the outer barrier heights, these certainly have some of the qualitative trends discussed in Section 2.4 and lend support to the feeling that, with renormalization to the quantitative level of the experimental results and shift of the neutron number centroid, the theory could be used to extrapolate fission barriers for unmeasured nuclei. Fig. 31 also shows a distinct odd-even effect in barrier heights, and this can be explained within the context of the Strutinsky theory; single particle level densities are high at the inner barrier and low at the minima (this is the basic mechanism for the double-humped barrier), so the energy gaps for even nuclei vary accordingly and must be reflected in the difference between the barrier heights relative to the ground states for even and odd nuclei. The penetrability parameters,  $\hbar \omega_A$ ,  $\hbar \omega_B$ , also show an odd-even effect, which can be qualitatively explained by the specialisation energy required to be added to the deformation energy for the 0<sup>+</sup> even-nucleus ground state in order to form the barrier for any other given spin and parity.

Overall, this general parametrisation for calculating the cross-sections of actinide nuclei, based on physical ideas arising from the theory of fission and other nuclear reaction processes but with actual parameters adjusted to key experimental data, appears to be successful at the level of confidence required for very many transactinium nuclei. The degree of confidence that can be placed on calculations of cross-sections of a statistical or 'integral' character (i.e. capture, summed inelastic scattering etc.) is of the order of 25 to 30% (in the sense of one standard deviation). A typical example is shown in Fig. 32; this is the capture cross-section of  $^{233}$ U compared with available experimental data [79,80]. One of the major factors entering this calculation is the competition from fission. The fission barriers were deduced from fission cross-section and sub-barrier (d,pF) fission probability data, low-lying levels in  $^{233}$ U for inelastic scattering were taken from experimental compilations, but all other parameters belonged to the general scheme of [67].

#### 6. Recommendations for 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 parametrisation 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 Möller [12] on the one hand, suggesting that the outer barrier is itself split giving a shallow third minimum, and of Larsson et al [14] 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 barrier 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 [82]), need to be extended to high excitation energies so that  $(n, \infty n)$  and  $(n, \infty nF)$  cross-sections can be treated with confidence. Barrier penetrability formulae need further consideration; the Hill-Wheeler formula eq. (31) is almost certainly too simple, and further work along the lines of the two-dimensional fission barrier models of Hofmann [83] and Massmann et al [84] 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 summarised in ref. [81].

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, yet these data are important for an understanding of fast reactor physics relating to such matters as breeding ratios and D&ppler 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 (see Section 4.1). 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 analyses of the great body of experimental data on neutron and gamma-ray emission in the fission process.

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Table 1. Comparative results on fission barrier heights from a range of calculations. The barrier heights are quoted in MeV relative to the primary minimum of the potential energy curve. For comparison with experimental data (normally quoted relative to the nuclear ground state) a zero-point beta-vibration energy should be subtracted from these numbers.

Reference	Remarks on calculation	V <sub>A</sub> ( <sup>240</sup> Pu)	V <sub>A</sub> ( <sup>244</sup> Pu)	V <sub>A</sub> ( <sup>232</sup> Th)	V <sub>B</sub> ( <sup>232</sup> Th)
Möller and Nix [12]	Folded Yukawa shell- model. No axial asymmetry in deformation but reflection asymmetry allowed.	5•45	6•3	2.9	5•7
Möller and Nix [12]	Modified harmonic- oscillator shell- model. No axial asymmetry but reflection asymmetry allowed.				8.0
Larsson and Leander [18]	Modified harmonic oscillator shell model. No axial asymmetry.	6•3	7•1	4•7	
Larsson and Leander [18]	Modified harmonic oscillator shell model. Axial asymmetry allowed.	5•6	5•9	4.7	
Flocard et al [21]	Hartree-Fock calculation. No axial asymmetry or reflection asymmetry. Pairing interaction strength proportional to surface area.	9•0			
Flocard et al [21]	Ditto, but pairing interaction strength constant.	11.0			

## Figure Captions

- Fig. 1 Schematic diagram of Strutinsky shell-correction method.
- Fig. 2 Nuclear energy calculated as a function of deformation (for cylindrically symmetric shapes) for <sup>240</sup>Pu using Strutinsky's prescription. Arrow on outer barrier, B, gives lowering of barrier as calculated from reflection asymmetric deformation. Calculation from Nix [3].
- Fig. 3 Energy levels of a harmonic oscillator potential for prolate spheroidal deformations. Numbers in diagram are numbers of particles filling the shell. From Nix [3].
- Fig. 4 Comparison of two different technical procedures for calculating the Strutinsky shell-correction energy from the same set of shell-model levels. The solid curve is calculated using the normal energy-averaging procedure for every specific deformation. The dashed curve is from the summing of smoothed energy levels fitted to the actual shell model levels over a large range of deformation. Diagram from ref. [5].
- Fig. 5 Binding energy of <sup>240</sup>Pu as function of deformation (the parameter Q is the quadrupole moment of the matter density) calculated with a Hartree-Fock method by Flocard et al [7]. Dashed and solid curves correspond to pairing-interaction strength independent of nuclear surface area and proportional to surface area respectively.
- Fig. 6 Potential energy landscapes for  $^{236}$ Th and  $^{250}$ Cm as calculated in ref. [18]. The plane is one of nuclear elongatior ( $\varepsilon$ ) versus axial asymmetry (Y). The nuclear shape is chosen so that the energy is minimised as a function of the hexadecapole deformation parameter  $\varepsilon_4$ . Energy contours are at intervals of 0.2 MeV. The heavy solid line with arrows follows roughly the track of minimum potential energy with increasing elongation through barrier A and secondary well II.
- Fig. 7 Inner barrier height as calculated from Strutinsky theory with a modified harmonic oscillator shell model with and without the axial asymmetry degree of freedom. Pairing interaction strength was assumed proportional to surface area, and the liquid-drop neutron-proton asymmetry constant  $k_s = 1.78$ . From ref. [18].
- Fig. 8 Calculated energy of second minimum using Strutinsky theory with modified harmonic oscillator shell-model potential. The liquiddrop neutron-proton asymmetry constant  $k_{c} = 2.8$ . From ref. [12].
- Fig. 9 Calculated outer barrier heights using modified harmonic-oscillator shell-model potential. From ref. [12].
- Fig. 10 Calculated fission barrier potential energy curves, using folded Yukawa shell-model potential. From ref. [12]. The dashed curves assume reflection symmetry in the nuclear shape, but the solid curves allow for minimization of the potential with respect to reflection asymmetry.

Fig. 11 Potential energy surface for <sup>210</sup>Po. From ref. [22].

Fig. 12 Potential energy surface for <sup>236</sup>U. From ref. [22].

- Fig. 13 Potential energy contours as function of volume ratio for range of values of neck radius of fissioning nucleus <sup>252</sup>Fm. The neck radius of 5 fm corresponds to the outer saddle point. From ref. [22].
- Fig. 14 Potential energy contours as function of volume ratio for range of values of neck radius of fissioning nucleus 256Fm. From ref. [25].
- Fig. 15 Potential energy contours as function of volume ratio for range of values of neck radius of fissioning nucleus 258Fm. From ref. [22].
- Fig. 16 Experimental data on mass yields from thermal neutron induced fission of 255Fm and 257Fm. From ref. [26].
- Fig. 17 Mass yield in thermal neutron-induced fission of <sup>255</sup>Fm for specific values of the total kinetic energy of the fission products. From ref. [26].
- Fig. 18 Potential energy surfaces as functions of mass asymmetry ratio and distance mass centres for 236U and 258Fm. From ref. [12].
- Fig. 19 Inertial parameter B corresponding to the collective parameter for nuclear c elongation, c, compared to the shell correction energy E shell. From ref. [36].
- Fig. 20 Least action trajectory for ground-state spontaneous fission of <sup>240</sup>Pu through potential energy landscape in plane of elongation parameter c and neck constriction, h. From ref. [36].
- Fig. 21 Least action calculations of ground-state spontaneous fission half-lives with optimised adjustments of surface energy constants for different groups of elements. From ref. [36].
- Fig. 22 Least action calculation spontaneously-fissioning isomer half-lives. From ref. [36].
- Fig. 23 Calculated single-particle neutron level schemes at the deformation of the second minimum, calculated for different shell-models by different authors. From ref. [42].
- Fig. 24 Calculated moment of inertia of the lowest rotational for <sup>240</sup>Pu as function of elongation c. From ref. [36].
- Fig. 25 Fission cross-section of <sup>230</sup>Th. From ref. [37].
- Fig. 26 Fission cross-section of <sup>237</sup>Np. Note change of scale at 100 eV. From ref. [47].
- Fig. 27 Results of dynamical calculation (bottom curves compared with experimental data) of mass yield for spontaneous fission of 2360 from Schrodinger equation in mass asymmetry variable at two different elongations (\_\_\_\_\_\_ overall length of nucleus = 1.8 x spherical diameter, --- 1.65 x spherical radius). Upper diagram shows inertial parameter and centre diagram shows potential energy. From ref. [48].
- Fig. 28 Statistical theory calculation of position of heavy mass-yield peak, its full-width at half-maximum and ratio R of peak-to-valley ratio for <sup>240</sup>Pu. Calculations from ref. [52], experimental data from [54].

Fig.	29	Thermodynamic theory calculation of deformation energy as
		function of volume asymmetry for various values of neck radius
		and internal excitation temperature. From ref. [56].

- Fig. 30 Intrinsic level densities for <sup>240</sup>Pu at deformations corresponding to the ground state and the inner barrier. From ref. [75].
- Fig. 31 Inner barrier heights of actinide nuclei determined from analysis of experimental data as function of mass number A. Open symbols denote even nuclei, hatched symbols denote odd-A nuclei and blocked symbols denote odd nuclei.
- Fig. 32 Calculated neutron capture cross-section of <sup>233</sup>U compared with experimental data.



FIG.1.

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FIG. 2





DEFORMATION &

FIG.4



MASS QUADRUPOLE MOMENT Q (BARNS)

FIG.5



824



E24

FIG. 6.



FIG. 7



FIG. 8



F(G.9



FIG. 10



FRAGMENT MASSES (amu)

FIG. 11.





FIG. 12.

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FIG. 13



FIG.14.



FIG.15







FIG. 18.







FIG. 23



FIG. 24





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FIG. 27

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Figure 28



Figure 29





MASS NUMBER A



Neutron Energy (MeV)

Figure 32