Springer Proceedings in Physics 254

Jutta Escher · Yoram Alhassid Lee A. Bernstein · David Brown Carla Fröhlich · Patrick Talou Walid Younes *Editors*

Compound-Nuclear Reactions

Proceedings of the 6th International Workshop on Compound-Nuclear Reactions and Related Topics CNR*18

Springer Proceedings in Physics

Volume 254

Indexed by Scopus

The series Springer Proceedings in Physics, founded in 1984, is devoted to timely reports of state-of-the-art developments in physics and related sciences. Typically based on material presented at conferences, workshops and similar scientific meetings, volumes published in this series will constitute a comprehensive up-todate source of reference on a field or subfield of relevance in contemporary physics. Proposals must include the following:

- − name, place and date of the scientific meeting
- − a link to the committees (local organization, international advisors etc.)
- − scientific description of the meeting
- − list of invited/plenary speakers
- − an estimate of the planned proceedings book parameters (number of pages/articles, requested number of bulk copies, submission deadline).

More information about this series at <http://www.springer.com/series/361>

Jutta Escher • Yoram Alhassid • Lee A. Bernstein David Brown • Carla Fröhlich • Patrick Talou Walid Younes **Editors**

Compound-Nuclear Reactions

Proceedings of the 6th International Workshop on Compound-Nuclear Reactions and Related Topics CNR*18

Editors Jutta Escher Lawrence Livermore National Laboratory Livermore, CA, USA

Lee A. Bernstein Lawrence Berkeley National Laboratory Berkeley, CA, USA

Carla Fröhlich North Carolina State University Raleigh, NC, USA

Walid Younes Lawrence Livermore National Laboratory Livermore, CA, USA

Yoram Alhassid Department of Physics Yale University New Haven, CT, USA

David Brown National Nuclear Data Center Brookhaven National Laboratory Upton, NY, USA

Patrick Talou Los Alamos [Nati](https://orcid.org/0000-0002-0536-3615)onal Laboratory Los Alamos, NM, USA

ISSN 0930-8989 ISSN 1867-4941 (electronic) Springer Proceedings in Physics
ISBN 978-3-030-58081-0 ISBN 978-3-030-58082-7 (eBook) <https://doi.org/10.1007/978-3-030-58082-7>

© This is a U.S. government work and not under copyright protection in the U.S.; foreign copyright protection may apply 2021

All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors, and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Preface

This volume contains the Proceedings of the 6th International Workshop on Compound-Nuclear Reactions and Related Topics (CNR*18), held at the Lawrence Berkeley National Laboratory, in Berkeley, California, on September 24–28, 2018.

The CNR* series began in 2007 with a meeting near Yosemite National Park. It has since been held in Bordeaux (2009), Prague (2011), Sao Paulo (2013), and Tokyo (2015). The workshop series focuses on improving our understanding of

reactions that involve compound nuclei. Even though the concept of the compound nucleus dates back to the 1930s, interest in compound-nuclear reactions, which exhibit a rich set of phenomena, remains strong. Statistical, semi-classical, and quantum mechanical approaches are employed to describe the static properties of the many-body systems and the dynamics of their collisions and decays. Traditional stable-beam and state-of-the-art radioactive-beam experiments, innovative indirect methods, and decay experiments are utilized to shed light on the reaction dynamics and relevant structural properties. Compound-nuclear reactions play a crucial role for applications in various areas, such as nuclear astrophysics, medicine, nuclear energy, and national security. An overarching goal of the series is to establish a comprehensive, quantitative picture of the processes involved in the formation and decay of a compound nucleus, informed and tested by appropriate experiments, and to formulate accurate predictions for the associated cross sections.

The CNR*18 workshop brought together experts in nuclear theory, experiment, and data evaluation. A broad range of topics was discussed: A number of presentations were dedicated to nuclear structure properties needed for the description of compound-nuclear reactions, such as level densities and gammaray strength functions. Other presentations addressed the reaction mechanisms associated with the formation and decay of compound nuclei, including preequilibrium processes, fluctuation effects, and possible deviations from standard statistical descriptions. Widely used codes for the description of compound-nuclear reactions were compared. Current efforts in improving optical models, R-matrix descriptions, and ab initio reaction theory were presented. Recent progress in developing indirect approaches for determining compound-nuclear cross sections, including the surrogate reactions method and the Oslo method, was reviewed. Theoretical approaches to fission, as well as experimental fission studies, were covered. Several presentations focused on nuclear astrophysics and on isotope production for medical applications. Overviews of existing and planned facilities for experimental studies of compound-nuclear reactions were presented. These Proceedings, edited by the CNR*18 organizing committee, contain summaries of the individual contributions presented at the workshop.

CNR*18 was organized by Jutta Escher and Walid Younes (Lawrence Livermore National Laboratory, LLNL), Yoram Alhassid (Yale University), Lee A. Bernstein (Lawrence Berkeley National Laboratory, LBNL), David Brown (Brookhaven National Laboratory, BNL), Carla Fröhlich (North Carolina State University), and Patrick Talou (Los Alamos National Laboratory, LANL). We thank Tom Gallant (LBNL) for his dedication and outstanding administrative assistance before, during, and after the workshop. We acknowledge support for the organization of the workshop and the publication of these Proceedings, provided by LLNL, LANL, BNL, LBNL, and the Nuclear Science and Security Consortium (NSSC). We would like to express our appreciation to the members of the international advisory committee for valuable suggestions regarding the program and to the session chairs

Preface viii and the contract of the contract

and panel members for providing a framework for inspiring discussions. We thank the participants for their positive response to the workshop, their extensive work and excellent presentations during the meeting, and their contributions to this volume.

Livermore, CA, USA Jutta Escher

New Haven, CT, USA Storm Alhassid New Haven, CT, USA Yoram Alhassid
Berkelev, CA, USA Lee A, Bernstein Berkeley, CA, USA Lee A. Bernstein

Upton, NY, USA David Brown Upton, NY, USA Raleigh, NC, USA Carla Fröhlich

Los Alamos. NM. USA Patrick Talou Los Alamos, NM, USA Patrick Talou

Livermore. CA. USA Patrick Talou

Walid Younes Livermore, CA, USA

Organization

Organizing Committee

International Advisory Committee

Contents

[Part III Optical Models](#page--1-0)

[Part VI Oslo Method](#page--1-0)

Part I Modeling Compound-Nuclear Reactions

Towards More Predictive Nuclear Reaction Modelling

S. Hilaire and S. Goriely

1 Introduction

Nuclear reaction models, beyond the fundamental quest for understanding processes taking place when a nuclear reaction occurs, are necessary to produce nuclear data for various applications. Depending on the targeted goal, the accuracy of the predictions as well as the type of data predicted might be very different. For nuclear reactors, for instance, the accuracy is clearly a key issue for specific nuclei and specific types of data. At the other extreme, one finds nuclear astrophysics for which the accuracy is less crucial than the ability of the model to produce data for all possible interacting systems. Even for the most important nuclei, for which many measurements have been performed, the need for better nuclear reaction models is still relevant since one still have to deal with processes for which data are not available or not precise enough. Within this context, nuclear reaction models have to be as robust and predictive as possible. This is why during the last 40 years at least, many nuclear reaction codes have been developed and used to answer the question: "what happens when a projectile hits a target nucleus?"

It is clear that the answer to this question depends on the nature of the projectile, on the target and on the projectile energy. In what follows, we restrict ourselves to the case where light projectiles (gamma, neutron, protons*...* up to 4He) interact with a target nucleus heavy enough (typically with a mass $A > 10$) with an incident energy between 1 keV and 200 MeV, a framework enabling the implementations of the so-called statistical models. Within this framework, several models come

S. Hilaire (\boxtimes)

CEA, DAM, DIF, Arpajon, France e-mail: stephane.hilaire@cea.fr

S. Goriely

Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, Brussels, Belgium

in the U.S.; foreign copyright protection may apply 2021

J. Escher et al. (eds.), *Compound-Nuclear Reactions*, Springer Proceedings in Physics 254, https://doi.org/10.1007/978-3-030-58082-7_1

[©] This is a U.S. government work and not under copyright protection

into play. We will first describe in Sect. 2, general features observed when a nuclear reaction occurs at energies below 200 MeV, features that have motivated the introduction of several models that will be discussed in Sect. [3.](#page-17-0) In Sect. [4,](#page-20-0) we will discuss current developments on specific ingredients required by the reaction models as those related to fission, for instance. Finally, Sect. [5](#page-25-0) will draw conclusions and prospects.

2 General Features About Nuclear Reactions

For incident projectiles with energy between a few keV and 200 MeV impinging on a target nucleus, the typical outgoing particle spectrum displays three main domains as illustrated in Fig. 1. Two extreme regimes can be distinguished. For high outgoing energies, and forward angles, discrete peaks are observed and dominate the outgoing spectrum. Such processes correspond to fast interactions, also called "direct interactions", which take place in a timescale comparable to the time the

Fig. 1 Outgoing proton spectrum for a 62 MeV incident proton on a ⁵⁶Fe target. Colours are used to distinguish the three regions corresponding to the direct reactions described by the optical model (blue), the pre-equilibrium model (green) and the compound nucleus model (red)

projectile takes to cross the nucleus. For low outgoing energies, a typical evaporation spectrum is observed. In this case, it is usually assumed that the projectile has been absorbed in the target with which it has shared all its energy to form a compound system. This process, described by the so-called compound nucleus (CN) model, assumes to the first order of approximation, that the formation and decay of the CN are independent processes. This assumption explains that the emission spectrum looks very similar whatever the angle of emission is: the compound nucleus has lost memory of the way it has been created! This feature is characterized by angular distribution of emitted particle symmetric around 90◦. Between these two extreme situations, one finds, if the projectile energy is high enough, an intermediate process whose frontiers are less well defined: the so-called pre-equilibrium process. This last process has been historically less studied than the two others (mainly because contrary to the two previous ones, it can be neglected for low incident energies) and, therefore, the formalism which is employed to describe it is still subject to important debates and still offers room for significant improvements. To these three types of processes, correspond in practice three types of models which are linked together, as illustrated in Fig. 2, in order to produce many different types of nuclear data: the "optical model (OM)", the "pre-equilibrium model (PE)" and the "CN model". All these models need to be implemented in a nuclear reaction code aiming at producing useful information. As can be observed, the optical and pre-equilibrium models both yield an output (elastic, fission or inelastic data) and also provide the CN model with an input data (σ $_{Reaction}$, T_{li} or σ_{NC}).

Fig. 2 Sequence of nuclear models required to describe a nuclear reaction

3 Nuclear Models for Nuclear Reactions

The three nuclear reaction models whose qualitative features have been discussed above rely on various input data. The latter can either be directly measured or have to be deduced from other models. Two types of approaches can be distinguished. The first one, traditionally employed, is generally based on empirical expressions which can be easily fine-tuned to reproduce data. The more recently developed ones have benefited from the increase in computing power which enables today to provide microscopic models able to compete with the traditional approaches.

3.1 Basic Nuclear Structure Information

The most fundamental data required for a nuclear reaction is the mass of the various nuclei that can appear during a decay process. This knowledge is necessary to determine reaction thresholds and to compute the kinematic relations enabling laboratory to centre of mass frame transformations. Other quantities such as nucleus levels' excitation energies, spins and parities are also welcome and govern features such as angular distribution or decay selection rules. Another feature also interesting though not mandatory is the deformed or spherical nature of the target. This information is particularly useful to adopt the proper treatment of the OM. Experimental nuclear masses are available today for nearly 2500 nuclei [\[1\]](#page-26-0). This set constitutes the reference data that nuclear mass models try to reproduce at best. Many different mass models have been developed during the last decades and the most advanced ones are able today to reach a root mean square (rms) deviation from experiment close to 500 keV [\[2\]](#page-26-0), a remarkable level of accuracy with respect to the mass of a nucleus of the order of a GeV. Generally speaking, the more the nuclear mass models are based on first principle physics, the higher the predictive power should be. This has been recently demonstrated by analysing the predictive power of various mass models adjusted on the 2003 atomic mass evaluation [\[3\]](#page-26-0) with respect to the update of 2012 [\[4\]](#page-26-0) and 2016 [\[1\]](#page-26-0). One of the big advantages of the microscopic models is that on top of the nuclear masses, they can also provide spectroscopic data, as well as all detailed input which can be used in other models, thus improving the coherence in an attempt to predict microscopically a nuclear reaction.

3.2 The Optical Model

The OM is very important since it determines the reaction cross section that the PE and CN models are then going to spread in the different outgoing open channels. It also provides the direct elastic, total and inelastic cross sections as well as various

angular distributions. Historically, the OM has been first determined postulating functional forms whose parameters have to be adjusted until a good agreement with data is obtained. This type of approach is still currently used [\[5\]](#page-26-0) in particular because of its ability to allow very accurate description of experimental data (less than 1% accuracy on total cross sections). However, it depends very much on experimental data availability. An alternative to the pure phenomenological approach is the microscopic approach. Such approaches enable to determine the OM without any a priori knowledge of any related experimental data. Therefore, it enables predictions even for nuclei far from the valley of stability. The disadvantage of such microscopic approaches is of course a lower accuracy. One of the most employed one is the socalled JLM approach [\[6\]](#page-26-0) which is based on nuclear matter data obtained from mean field or beyond mean field nuclear structure descriptions. Such structure methods generally provide a nuclear structure description which is hoped to be precise enough to guaranty that predictions far from the valley of stability should not be too far from the reality.

The choice between phenomenology and microscopy is guided by the goal one has in mind. Within the framework of nuclear data evaluation where accuracy is one of the key issues, availability of experimental data will make it preferable to use the first option because of its fitting power. For more fundamental research or when there is a lack of data, the microscopic option is preferred.

3.3 The Pre-equilibrium Model

Once the OM has treated the various direct processes, the remaining cross section, corresponding to all processes which have not been explicitly accounted for, is "feeding" the second model of Fig. [2,](#page-17-0) the PE model. This reaction cross section reflects the probability that the projectile be captured in the continuum of the target to form a "composite" system. At this stage, the system still remembers the way it was formed and is going to de-excite either by re-emitting a particle or by distributing step by step the incident projectile energy between one or several nucleons of the target. In the latter case, several particles and holes are going to be created sequentially, holding on towards more complex configurations, to reach, after sufficient time, a situation corresponding to the CN approximation, where the projectile energy has been shared among all the constituents of the composite system. At each step of this process, the probability to emit a particle has to be accounted for. Again, one has the choice between more or less refined models. The most employed one is the so-called exciton model, introduced in the seventies, which has been successively improved to account for more and more physical features either because the appearance of new experimental data evidenced a lack of predictive power or simply because initially missing, though important, features were introduced [\[7\]](#page-26-0). Quantum mechanical approaches have also been developed but they are clearly more complex and less flexible and do not provide results of better quality as those obtained with the exciton model. However,

recent experimental measurements seem to show that such quantum mechanical approaches are unavoidable if one aim at improving the predictive power [\[8\]](#page-26-0).

3.4 The Compound Nucleus Model

Beyond the fact that optical and pre-equilibrium models contribute to the emission of particles, they are also those which determine the initial conditions of the last model of the chain of Fig. [2:](#page-17-0) the CN model. Starting from such initial conditions, the CN model then uses the statistical hypothesis stating that the decay in a given outgoing channel depends on the ratio of the probability to decay in this specific channel with respect to all possible decay probabilities. This approximation, which consists in considering that the decay of the CN does not keep track of the CN formation (the Bohr hypothesis), is formally translated into the so-called Hauser– Feshbach equation,

$$
\sigma_{ab} = \sum_{J,\pi} \sigma_a^{NC} (E*, J, \pi) \frac{\langle \Gamma_b (E*, J, \pi) \rangle}{\sum_c \langle \Gamma_c (E*, J, \pi) \rangle}
$$

In this equation, σ_{ab} , corresponding to the cross section for the decay in channel *b* (particle type, energy, outgoing angular momentum) from the compound nucleus formed in the entrance channel a, is given by the product of the CN formation cross section σ_a^{NC} at a given energy, spin and parity (E^*, J, π) by the probability to decay in channel *b* given all open channels *c*. The question, therefore, consists in estimating all possible average decay widths Γ_c . The Hauser–Feshbach approximation enables to write, to the first-order approximation, that

$$
\frac{\langle \Gamma_b (E*, J, \pi) \rangle}{\sum_c \langle \Gamma_c (E*, J, \pi) \rangle} = \frac{\langle T_b^{J\pi} (E*) \rangle}{\sum_c \langle T_c^{J\pi} (E*) \rangle},
$$

where the transmission coefficients $\langle T_c \rangle$, which will be further discussed in Sect. 4, correspond to the decay probability in outgoing channel *c* (note that this expression becomes much more complicated when spin and parity conservation rules are explicitly written). Soon, it was realized that this first-order approximation had to be corrected at low energy, or, more precisely when the number of competing channel is relatively low. In such situations, indeed, interferences, either constructive or destructive, occur between entrance and exit channels. These interferences are accounted for introducing a width fluctuation correction factor, which, generally enhances the elastic channel and accordingly decreases the other competing channels [\[9\]](#page-26-0), but can also, in very particular situation, enhance the first inelastic channel [\[10\]](#page-26-0).

4 Nuclear Reaction Model Ingredients

The models described in the previous section require specific ingredients depending on the outgoing channel under consideration. To be more precise, the OM only provides transmission coefficient for outgoing particle decay to a well-defined level of the residual nucleus. However, it does not enable to deal with the particle decay in the residual nucleus levels' continuum, with photon emission, and does not provide either any fission decay probability. These three situations require supplementary particular approximations that we now discuss.

4.1 Particle Decay in the Continuum

When the projectile energy is large enough, the compound nucleus can decay by emitting a particle in the residual levels' continuum. This continuum has to be accounted for because it is well known that beyond a given excitation energy it is impossible to describe nuclear excited levels individually. In such cases, a nuclear level density (NLD) has to be introduced and the transmission coefficients entering the Hauser–Feshbach expression are given by the integral

$$
\left\langle T_c^{J\pi} \left(E_c \right) \right\rangle = \int_{E_c - \Delta}^{E_c + \Delta} \rho \left(\varepsilon \right) T_c^{J\pi} \left(E_c \right) d\varepsilon
$$

in which E_c is the excitation energy of the residual nucleus once a particle has been emitted in a channel *c*, $\rho(\varepsilon)$ the residual nucleus level density in which we have omitted, for simplicity, the spin and parity labels which are implicitly included in the definition of the channel c and Δ is the width of the excitation energy bin into which the emission occurs. An extensive literature exists on nuclear level densities, where both analytical and microscopic approaches are considered. Analytical approaches, because of the free parameters they contain allow one to fit both low energy levels and experimental s-wave mean spacings rather well [\[11\]](#page-26-0). Concerning the microscopic alternatives, one has to find a compromise between accuracy and completeness. The most advanced approaches [\[12\]](#page-26-0) are usually limited to local mass regions, and, so far only few approaches have been used to provide complete sets of data for all nuclei [\[13,](#page-27-0) [14\]](#page-27-0). The main advantage of the microscopic approaches is that they usually go beyond the assumed statistical hypothesis used in analytical expressions, a feature that can have a significant impact when comparing theoretical and experimental cross sections [\[15\]](#page-27-0).

As illustrated in Fig. [3,](#page-22-0) for instance, the combinatorial level density approach predicts much more high spin levels than the statistical approach (right panel), and such differences strongly modify the isomer production by photo-neutron reaction on 181 Ta (left panel).

Fig. 3 (Left) $181 \text{Ta}(\gamma, n)$ and $181 \text{Ta}^m(\gamma, n)$ cross sections. (Right) Level density ratio for specific spins. In the left panel, the use of the combinatorial level density predictions (full line) improves the description of the isomer production with respect to the results obtained using the statistical (dotted line). See Ref. [\[15\]](#page-27-0) for more details

4.2 Photon Emission

Whatever the projectile energy, γ emission is always an open decay channel for which the residual nucleus turns out to be the compound system with a lower excitation energy, the difference being the energy of the emitted photon. To determine a γ transmission coefficient, one assumes that photo-absorption and photoemission cross sections associated with a given decay type $X(X = E$ or M for electric or magnetic transition) and a given multipolarity are related one with the other, thanks to the same so-called photon strength function (PSF). Experimentally, the PSF follows a Lorentzian shape, whose parameterization can be more or less complicated [\[16\]](#page-27-0). A specific feature of the capture process is due to the fact that the γ decay occurs from the continuum of the CN to a very large number of levels, therefore requiring, the use of a NLD to be modelled, and, on top of that, the PSF concerns low-energy photons in the tail of the Lorentzian which cannot be constrained by photo data. One has then two sources of uncertainty which are combined to produce a total γ -ray transmission coefficient. For this reason, the theoretical γ -ray width is often quite different from the measured one, and a renormalization factor is introduced in the PSF to improve the agreement with either the measured γ -ray width or the experimental capture cross section data. Microscopic alternatives have been developed [\[17,](#page-27-0) [18\]](#page-27-0) and have shown significant deviations from the Lorentzian shape as far as the PSF is concerned, in particular for nuclei far from the valley of stability [\[17\]](#page-27-0). Quite recently, attempts to solve the normalization problem have also been undertaken [\[19,](#page-27-0) [20\]](#page-27-0). The current situation reached within the Gogny-QRPA framework is illustrated in Fig. [4.](#page-23-0) As can be observed, the agreement with experimental radiative widths is much better with the microscopic approach provided a phenomenological correction is used to describe the de-excitation PSF at low γ -emission energies [\[20\]](#page-27-0). It is worth adding that on

Fig. 4 Average radiative widths as function of the mass number. Comparison between theoretical predictions and experiment. The (**a**) and (**b**) panels correspond to the traditional analytical expression SLO and GLO [\[16\]](#page-27-0), while panels (**c**) and (**d**) display the HFB-Gogny QRPA predictions with two options for the low energy M1 phenomenological correction [\[20\]](#page-27-0)

top of its ability to reproduce experimental radiative width, the HFB-Gogny QRPA model has also been tested successfully with respect to other experimental data [\[21,](#page-27-0) [22\]](#page-27-0).

4.3 Fission

Despite its fundamental role in nuclear applications as a source of energy, as well as the fact that it has been discovered many decades ago and intensively studied since, fission remains probably the least well-understood process in nuclear reaction modelling. Qualitatively speaking, fission is modelled by a gradual transition of the nucleus from an initial compact shape to such an elongated shape that the nucleus breaks into fragments. This evolution is governed by a potential energy landscape corresponding to nuclear shapes more or less probable depending on the excitation energy required to reach them. This landscape exhibits features such as valleys and peaks which help in understanding the major characteristics of the fission process, and, in particular the fission fragments distributions observed experimentally. For cross section calculation, one reduces the multidimensional landscape to an effective one-dimensional (1D) approach. This 1D landscape suggests the concept of fission barriers through which quantum tunnelling probabilities are computed to determine fission transmission coefficients.

Given an initial compound nucleus state, fission occurs by tunnelling through all accessible fission barriers. Therefore, for a single barrier, the fission transmission coefficient is given by

$$
T_f(E, J, \pi) = \sum_{d(J, \pi)} T_{hw} (E - \varepsilon_d) + \int_{E_c}^{E + B_n} \rho(\varepsilon, J, \pi) T_{hw} (E - \varepsilon) d\varepsilon
$$

in which ε corresponds to the transition states' energies. These transition states are discrete up to a given arbitrary threshold *Ec*, and, as for the compound nucleus at normal deformation, are then described by a NLD, $ρ(ε, J, π)$, beyond E_c .

The potential energy surface often displays several barriers and the fission transmission coefficient used in the Hauser–Feshbach model takes more complicated forms [\[23–25\]](#page-27-0). For multiple humped fission barriers, one also accounts for the fact that there exist potential wells between the barriers in which quantum states can be located, usually called class-II or class-III states depending upon whether they are located between the first and second barrier or between the second and the third. If these class-II/III states have a spin and parity corresponding to that of the compound nucleus from which fission occurs, they induced a resonance effect in the fission transmission coefficient for which more or less refined treatments are possible [\[23–](#page-27-0) [25\]](#page-27-0).

When one uses traditional (i.e. based on analytical expressions) methods to compute fission cross section, a large number of parameters have to be adjusted to reproduce at best experimental data. One can adjust the fission barrier heights and widths, the transition states and their corresponding NLD parameters as well as the eventual class-II/III states. With increasing kinetic energy of the projectile, several residual nuclei come into play. For a 10 MeV neutron incident on 238 U, for instance, both 239 U (first-chance fission) and 238 U (second-chance fission) fission barrier parameters have to be simultaneously fine-tuned and the higher the incident energy, the larger the number of fissioning nuclei. If this makes the fine-tuning more complicated, it also provides a way to get more constraints than the single 238 U neutron-induced fission cross section, provided one wants to coherently model the several fission chances.

To be more precise, the fact that the fourth chance of 238 U fission is governed by the fission barriers of 236 U implies that the latter should also provide a good description of the first chance of 235 U since in both cases the nucleus which undergoes fission is the same. Another constraint can also be obtained by noticing that the fission barriers parameters enabling a proper description of photo-induced fission on 238U should also provide a good second-chance fission of neutron-induced fission of ²³⁸U. Therefore, a coherent modelling of fission means that the same set of input parameters should provide simultaneously the various fission chances of the various fissioning systems encountered within a given isotopic chain. An illustration of the results obtained within such a modelling framework is given in Fig. [5.](#page-25-0) If the price to pay by considering all these constraints is an important amount of work, the reward is a simultaneous description of a whole isotopic chain. In the case of 238 U neutron-induced fission indeed, fitting experimental fission cross section data up to 40 MeV requires to adjust the fission parameters for all Uranium isotopes between 239 U (first-chance fission) and 235 U (fifth chance) as well as other fission chances due to the opening of proton emission and 4 He emission (see Fig. 5). Semimicroscopic alternatives to such a modelling framework have been studied and have shown promising results [\[26,](#page-27-0) [27\]](#page-27-0). Even though the accuracy reached is not at the level required for practical applications, this is a direction to follow in particular if one aims at studying fission for nuclei far from experimentally accessible regions.

Fig. 5 Illustrations of the coherent modelling of fission cross sections. (**a**) Neutron-induced fission cross section on 238U. (**b**) Neutron-induced fission cross section on 237U. (**c**) Neutron-induced fission cross section on 236 U. (**d**) Neutron-induced fission cross section on 235 U. In panel (**a**), the vertical lines indicate for which incident neutron energy new fissioning nuclei have to be accounted for (see text for more explanations). These fissioning systems are indicated in red as well as the emission process they are involved in

5 Conclusions

The modelling of a nuclear reaction is a complicated task, sometimes challenging. Several models and nuclear ingredients have to be linked together to be able to predict the outcome of a nuclear reaction. Although significant improvements have been made during the last decades, there are still many challenges to face. Pre-equilibrium and fission modelling are certainly among these. In the case of pre-equilibrium, the main reason is that the flexibility of semi-classical approaches makes it possible to obtain at small computational price results which satisfy the quality required for applications. It is only recently that the need for better models has become timely, in particular while studying "subtle" processes such as (*n,xn*γ) transitions in actinides [8]. For fission, the problem is more complicated. The models used are far too simple compared to the most fundamental approaches which evidence a need to account for multidimensional energy landscapes. If future developments consist, without any doubt, in adding more and more microscopic approaches in the nuclear reaction models, this will be a very long-term project. For now, such microscopic approaches can only provide guidelines for nuclear data evaluations but offer the only alternative to empirical expressions whose predictive power far from the valley of stability cannot be trusted given the number of phenomenological parameters they rely on.

References

- 1. G. Audi et al., The NUBASE 2016 evaluation of nuclear properties. Chin. Phys. C **41**(3), 030001 (2017)
- 2. A. Sobiczewski, Y. Litvinov, Predictive power of nuclear-mass models. Phys. Rev. C **90**, 017302 (2014)
- 3. G. Audi et al., The AME2003 atomic mass evaluation. Nucl. Phys. A **729**, 337–676 (2003)
- 4. G. Audi et al., The Ame2012 atomic mass evaluation. Chin. Phys. C **36**(12), 1287–1602 (2012)
- 5. A.J. Koning, J.P. Delaroche, Local and global nucleon optical models from 1 keV to 200 MeV. Nucl. Phys. A **713**, 231–310 (2003)
- 6. E. Bauge et al., Lane-consistent semi-microscopic nucleon-nucleus optical model. Phys. Rev. C **63**, 024607 (2001)
- 7. A.J. Koning, J.M. Akkermans, in *Workshop on Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety*, ed. by P. Oblozinsky, A. Gandini, (ICTP, Trieste, 1998), p. 143, Feb 23–March 27 1998
- 8. M. Dupuis et al., Microscopic modeling of direct pre-equilibrium emission from neutron induced reactions on even and odd actinides. EPJ Web Conf. **146**, 12002 (2017)
- 9. S. Hilaire et al., Comparison between various width fluctuation correction factors for compound nucleus reactions. Ann. Phys. **306**, 209 (2003)
- 10. T. Kawano et al., Statistical Hauser-Feshbach theory with width fluctuation correction including direct reaction channels for neutron induced reaction at low energy. Phys. Rev. C **94**, 014612 (2016)
- 11. A.J. Koning et al., Global and local level density models. Nucl. Phys. A **810**, 13–76 (2008)
- 12. Y. Alhassid, The shell model Monte Carlo approach to level densities: Recent developments and perspectives. Eur. Phys. J. A **51**, 171 (2015)
- 13. S. Hilaire et al., Temperature-dependent combinatorial level densities with the D1M Gogny force. Phys. Rev. C **86**, 064317 (2012)
- 14. S. Goriely et al., Microscopic nuclear level densities for practical applications. Nucl. Phys. A **695**, 95–108 (2001)
- 15. S. Goko et al., Partial photoneutron cross sections for the isomeric state ¹⁸⁰Ta^m. Phys. Rev. Lett. **96**, 192501 (2006)
- 16. R. Capote et al., Reference input parameter library for calculation of nuclear reactions and nuclear data evaluations. Nucl. Data Sheets **110**, 3107–3214 (2009)
- 17. S. Goriely et al., Microscopic HFB + QRPA predictions of dipole strength for astrophysics applications. Nucl. Phys. A **739**, 331–352 (2004)
- 18. M. Martini et al., Large-scale deformed quasiparticle random-phase approximation calculations of the gamma-ray strength function using the Gogny force. Phys. Rev. C **94**, 014304 (2016)
- 19. M.R. Mumpower et al., Estimation of M1 scissors mode strength for deformed nuclei in the medium- to heavy-mass region by statistical Hauser-Feshbach model calculations. Phys. Rev. C **96**, 024612 (2017)
- 20. S. Goriely et al., Gogny-HFB+QRPA dipole strength function and its application to radiative nucleon capture cross section. Phys. Rev. C **98**, 014327 (2018)
- 21. S. Goriely et al., Reference database for photon strength functions. Eur. Phys. J. A **55**, 172 (2019)
- 22. M. Krticka et al., Constraints on the dipole photon strength functions from experimental multistep cascade spectra. Phys. Rev. C **99**, 044308 (2019)
- 23. M.J. L Lopez Jiménez et al., Triple-humped fission barrier model for a new 238U neutron cross-section evaluation and first validations. Ann. Nucl. Energy **32**, 195 (2005)
- 24. P. Romain et al., Bruyères-le-Châtel neutron evaluations of actinides with the TALYS code: The Fission Channel. Nucl. Data Sheets **131**, 222 (2016)
- 25. M. Sin et al., Fission of light actinides: 232Th(n, f) and 231Pa(n, f) reactions. Phys. Rev. C **74**, 014608 (2006)
- 26. S. Goriely et al., Towards a prediction of fission cross sections on the basis of microscopic nuclear inputs. Phys. Rev. C **79**, 024612 (2009)
- 27. S. Goriely et al., Towards an improved evaluation of neutron-induced fission cross sections on actinides. Phys. Rev. C **83**, 034601 (2011)

Modeling Compound Nuclear Reactions with EMPIRE

M. Herman, R. Capote, B. V. Carlson, M. Sin, and A. Trkov

1 Introduction

The description of low-energy nucleon-induced reactions in the continuum region requires, at the very least, calculations of elastic scattering within the optical model and of statistical emission of photons and light particles from the compound nucleus formed from the fusion of the projectile and target. If actinide targets are to be described, a reasonably sophisticated model of fission should also be included in the statistical emission calculation. At very low energies, width fluctuation corrections must be included, while at energies above about 10 MeV, pre-equilibrium effects should be taken into account.

The EMPIRE code, [\[36\]](#page--1-0) first released in 1980, calculated both elastic scattering and the cross sections and spectra of statistical equilibrium and pre-equilibrium decay processes. It was later extended to include width fluctuation corrections to low-energy cross sections. A version for heavy-ion induced reactions was also introduced.

In its second release, EMPIRE-2, the code was entirely rewritten using a modular structure, as well as taking advantage of more relaxed memory limitations, to obtain an increase in execution speed of about a factor of 20. The new code was projected

M. Herman

R. Capote · A. Trkov

B. V. Carlson (\boxtimes)

M. Sin Faculty of Physics, University of Bucharest, Bucharest, Romania

© This is a U.S. government work and not under copyright protection in the U.S.; foreign copyright protection may apply 2021 J. Escher et al. (eds.), *Compound-Nuclear Reactions*, Springer Proceedings in Physics 254, https://doi.org/10.1007/978-3-030-58082-7_2

Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, USA

NAPC-Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria

Instituto Tecnológico da Aeronáutica, São José dos Campos, SP, Brazil

to be general and flexible. Each module was designed to perform a well-defined task and to communicate with other modules through a set of global COMMON blocks. This assured access to all the resources throughout the code and facilitated the addition of new features and mechanisms. The third release of the code, EMPIRE-3, maintains and extends this structure.

The current version, EMPIRE-3.2, is named Malta, after Napoleon's capture of the island on the way to Egypt. Although a minor release, it features a number of significant improvements such as: (1) prompt fission neutron spectra, including automatic adjustment to experimental data, (2) anisotropic angular distributions for compound elastic and inelastic excitations, (3) simulation of the Engelbrecht-Weidenmüller transformation, and (4) new IO subroutines for the manipulation of ENDF-6 formatted files.

2 Basic Objectives and Scope

The basic objectives of the EMPIRE code are:

- to provide the state-of-the-art modeling of nuclear reactions for basic science and data evaluation;
- to ensure reasonably comprehensive coverage of incident particles, targets, incident energies, and observables;
- To unify (1) reaction models, (2) model parameters, (3) nuclear structure data, and (4) experimental results;
- to provide a full set of tools for evaluators to enable efficient production of high quality nuclear data files;
- to be as general, flexible, and easy to use as possible.

The present scope of the code includes:

- A broad range of incident energies (up to 150 MeV) and projectiles (n, p, d, t, 3 He, 4 He, photons, and heavy ions);
- The low-energy range for neutron reactions covered by an interface to the Atlas of Neutron Resonances [\[1\]](#page--1-0);
- Default input parameters for targets of mass number $A \ge 20$ [\[2\]](#page--1-0);
- Direct, pre-equilibrium, and statistical model reaction mechanisms—with width fluctuations and a full gamma cascade;
- Observables: cross sections, angular distributions, spectra (including prompt fission neutron spectra), energy-angular distributions;
- Outgoing channels: multi-particle emission, *γ* -emission (including discrete lines), discrete levels (including isomers), fission, several exclusive channels.

To a large extent, the present scope of the EMPIRE code permits it to fulfill its objectives. However, it should also be clear that the objectives are an evolving target that will never be completely met.