Towards more accurate and reliable predictions for nuclear applications

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Abstract. The need for nuclear data far from the valley of stability, for applications such as nuclear astrophysics or future nuclear facilities, challenges the robustness as well as the predictive power of present nuclear models. Most of the nuclear data evaluation and prediction are still performed on the basis of phenomenological nuclear models. For the last decades, important progress has been achieved in fundamental nuclear physics, making it now feasible to use more reliable, but also more complex microscopic or semi-microscopic models in the evaluation and prediction of nuclear data for practical applications. In the present contribution, the reliability and accuracy of recent nuclear theories are discussed for most of the relevant quantities needed to estimate reaction cross sections and beta-decay rates, namely nuclear masses, nuclear level densities, gamma-ray strength, fission properties and beta-strength functions. It is shown that nowadays, mean-field models can be tuned at the same level of accuracy as the phenomenological models, renormalized on experimental data if needed, and therefore can replace the phenomenological inputs in the prediction of nuclear data. While fundamental nuclear physicists keep on improving state-of-the-art models, e.g. within the shell model or ab initio models, nuclear applications could make use of their most recent results as quantitative constraints or guides to improve the predictions in energy or mass domain that will remain inaccessible experimentally.

1 Introduction

Among the various field in nuclear astrophysics, nucleosynthesis is clearly the one the most closely related to nuclear physics, the nuclear physics imprint being found in the origin of almost all nuclides produced in the Universe [1]. Impressive progress has been made for the last decades in the various fields related to nucleosynthesis, especially in experimental and theoretical nuclear physics, as well as in ground-based or space astronomical observations and astrophysical modellings. In spite of that success, major problems and puzzles remain. In particular, experimental nuclear data only covers a minute fraction of the whole set of data required for nucleosynthesis applications. Reactions of interest often concern unstable or even exotic (neutron-rich, neutron-deficient, superheavy) species for which no experimental data exist. In addition, a large number (thousands) of unstable nuclei may be involved for which many different properties have to be determined (fig. 1). Finally, the energy range for which measurements are available is restricted to the small range reachable by present experimental setups. To fill the gaps, only theoretical predictions can be used.

Among the various nuclear astrophysics problems, one specific nucleosynthesis process remains extremely difficult to solve. It concerns the rapid neutron-capture process, or r-process, invoked to explain the production of the stable (and some long-lived radioactive) neutron-rich nuclides heavier than iron that are observed in stars of various metallicities, as well as in the solar system (for a review, see ref. [2]). In recent years, nuclear astrophysicists have developed more and more sophisticated r-process models, trying to explain the solar system composition by adding new astrophysical or nuclear physics ingredients. The r-process remains the most complex nucleosynthetic process to model from the astrophysics as well as nuclear-physics points of view. The site(s) of the r-process is (are) not identified yet, all the proposed scenarios facing serious problems. Complex — and often exotic— sites have been considered in the hope of identifying astrophysical conditions in which the production of neutrons is large enough to give rise to a successful r-process.

Progress in the modelling of type-II supernovae and γ-ray bursts has raised a lot of excitement about the so-called neutrino-driven wind environment [2–4]. However,
Fig. 1. (Color online) Schematic representation in the \((N, Z)\) plane of the different nuclear astrophysics applications, including nucleosynthesis processes, composition and structure properties of neutron stars. For each process, the nuclear needs are sketched. The open black squares correspond to stable or long-lived nuclei, the yellow squares to the nuclei for which masses have been measured and the blue square to those which may fission. See text for more details.

Until now a successful \(r\)-process has not been obtained \textit{ab initio} without tuning the relevant parameters (neutron excess, entropy, expansion timescale) in a way that is not supported by the most sophisticated existing models. Early in the development of the theory of nucleosynthesis, an alternative to the \(r\)-process in high-temperature supernova environments was proposed. It concerns the decompression of cold neutron star (NS) matter which was found to be favorable for strong \(r\)-processing [5].

Recently, special attention has been paid to NS mergers following the confirmation by hydrodynamic simulations that a non-negligible amount of matter, typically about \(10^{-3}\) to \(10^{-2}\)\(M_\odot\), can be ejected [6–13]. In contrast to the supernova site, investigations with growing sophistication have confirmed NS merger ejecta as viable sites for strong \(r\)-processing [2, 10–18]. In particular, recent nucleosynthesis calculations [13] show that the combined contribution of both the dynamical (prompt) ejecta expelled during the binary NS-NS or NS-black hole (BH) merger, as well as the neutrino and viscously driven outflows generated during the post-merger remnant evolution of the relic BH-torus systems lead to the production of \(r\)-process elements from \(A \gtrsim 90\) up to thorium and uranium with an abundance distribution that reproduce extremely well the solar distribution, as well as the elemental distribution observed in low-metallicity stars [19–21].

The ejected mass of \(r\)-process material, combined with the predicted astrophysical event rate (around 10\(\text{Myr}^{-1}\) in the Milky Way [22]) can account for the majority of \(r\)-material in our Galaxy [10, 11]. Recent studies [23–28] have also reconsidered the galactic or cosmic chemical evolution of \(r\)-process elements in different evolutionary contexts, and although they do not converge towards one unique quantitative picture, most of them got to the conclusion that double compact star mergers may be the major production sites of \(r\)-process elements.

In this specific \(r\)-process scenario, the number of free neutrons per seed nuclei can reach a few hundreds. With such a neutron richness, heavy fissioning nuclei can be produced. Thanks to this property, the final composition of the ejecta is rather insensitive to details of the initial abundances and the astrophysical conditions, in particular the mass ratio of the two NSs, the quantity of matter ejected, and the equation of state [10, 11, 18]. This robustness, which is compatible with the uniform, solar-like abundance pattern of the rare-earth elements observed in metal-poor stars [19–21], supports the possible creation of these elements by fission recycling in NS merger ejecta.

\(r\)-process nucleosynthesis calculations require a reaction network including about 5000 species from protons up to \(Z \approx 110\) lying between the valley of \(\beta\)-stability and the neutron drip line. All charged-particle fusion reactions on light and medium-mass elements that play a role when the nuclear statistical equilibrium freezes out need to be included in addition to radiative neutron captures and photodisintegrations. On top of these reactions, \(\beta\)-decays as well as \(\beta\)-delayed neutron emission probabilities and \(\alpha\)-decay rates need to be taken into account, but also fission processes, including neutron-induced, spontaneous, \(\beta\)-delayed and photofission, together with the corresponding fission fragment distribution (FFD) for all fissioning nuclei. All rates are based on experimental whenever available, but since only a extremely small amount of data are known experimentally, theoretical models are fundamental in providing the various predictions.

For such applications, the necessary ingredients (properties of cold and hot nuclei, nuclear level densities (NLD), optical potentials, \(\gamma\)-ray strength functions, fission properties, \(\beta\)-strength functions) should ideally be derived from \textit{global, universal} and \textit{microscopic} models. The large number of nuclides involved in the modelling of some nucleosynthesis mechanisms demands the use of global models.
On the other hand, a universal description of all nuclear properties within a unique framework for all nuclei involved ensures the essential coherence of the predictions of all unknown data. Finally, a microscopic description provided by a physically sound theory based on first principles ensures extrapolations away from experimentally known energy or mass regions that are likely to be more reliable than predictions derived from more or less parametrized approaches of various types and levels of sophistication. These include, between the extreme approaches provided by local macroscopic approaches and global microscopic ones, models referred to as classical, semi-classical, macroscopic-microscopic (e.g. classical with microscopic corrections), or semi-microscopic (e.g. microscopic with phenomenological corrections). Nowadays, microscopic models can be tuned to the same level of accuracy as the phenomenological models, and therefore could replace the phenomenological inputs in practical applications.

Today, due to our ignorance on the exact conditions in which the r-process takes place, it remains difficult to estimate the precision with which the various relevant rates need to be estimated. In particular, it strongly depends if an \((n,\gamma)-(\gamma,n)\) equilibrium would be reached during the neutron irradiation or if, instead, a competition between neutron captures and \(\beta\)-decays would be responsible for the nuclear flow and final shaping of the r-abundance distribution. Much more work on the astrophysical modelling [2] is needed before providing such constraints that could shed light on the precision required from nuclear physics. In the meantime, a first educated guess would require the reaction rates to be estimated within a factor of 2 and \(\beta\)-decay rates within 50% for all nuclei that may be direct progenitors of r-nuclei, i.e. before the final \(\beta\)-decay cascade at the neutron freeze-out. Concerning the more exotic nuclei up to the neutron drip-line, depending if fission efficiently recycles material, i.e. depending on the number of neutrons per seed available, less stringent constraints could be envisioned. It also remain of first importance to estimate the statistical as well as systematic uncertainties affecting the predictions far away from the experimentally known region. Such a difficult task has been started regarding mass predictions, but remains to be performed for the reaction as well as \(\beta\)-decay rates. Our capacity to predict the most important rates, i.e. the neutron capture (sect. 2), fission (sect. 3), \(\beta\)-decay (sect. 4) rates, is described in the present paper and the need to improve global, universal and microscopic models emphasized. Conclusions are drawn in sect. 5.

2 Radiative neutron captures

As far as reaction on heavier nuclei are concerned, most of the low-energy cross section calculations for practical applications are based on the statistical model of Hauser-Feshbach. Such a model makes the fundamental assumption that the capture process takes place with the intermediate formation of a compound nucleus (CN) in thermodynamic equilibrium. The energy of the incident particle is then shared more or less uniformly by all the nucleons before releasing the energy by particle emission or \(\gamma\)-deexcitation. The formation of a CN is usually justified by assuming that the level density in the compound nucleus at the projectile incident energy is large enough to ensure an average statistical continuum superposition of available resonances. The statistical model has proven its ability to predict cross sections accurately. However, this model suffers from uncertainties stemming essentially from the predicted nuclear ingredients describing the nuclear structure properties of the ground and excited states, and the strong and electromagnetic interaction properties. Our capacity to predict reliably all these ingredients, i.e. the nuclear structure properties (masses, deformations, matter densities), the NLD, the optical potential and the \(\gamma\)-ray strength function, especially for exotic neutron-rich nuclei, are discussed in the next subsections and their impact on the reaction cross sections illustrated (fig. 2). Additionally, the direct capture (DC) contribution may dominate the reaction mechanism, with respect to the CN statistical contribution, for exotic nuclei for which the number of available states in the CN is small. Some issues related to the DC are discussed in sect. 2.5.

2.1 Nuclear masses

Among the ground-state properties, the atomic mass is obviously the most fundamental quantity (for a review on atomic masses, see e.g. [29]). The calculation of the reaction cross section also requires the knowledge of other ground-state properties, such as the deformation, density distribution or the single-particle level scheme. When not available experimentally, these quantities need to be extracted from a mass model which aims at reproducing measured masses as accurately as possible, i.e. typically with a root-mean-square (rms) deviation of about 700 keV. The importance of estimating all ground-state properties reliably should not be underestimated. For example, the NLD of a deformed nucleus at low energies (typically at the neutron separation energy) is predicted to be significantly (about 30 to 50 times) larger than of a spherical one due principally to the rotational enhancement. An erroneous determination of the deformation can therefore lead to large errors in the estimate of radiative capture cross sections. For this reason, modern mass models not only try to reproduce at best experimental masses and mass differences, but also charge radii, quadrupole moments, giant resonances, fission barriers, shape isomers, infinite nuclear matter properties, etc...

With a view to their astrophysical application in neutron-rich environments, a series of nuclear-mass models have been developed recently based on the Hartree-Fock-Bogoliubov (HFB) method with Skyrme and contact-pairing forces, together with phenomenological Wigner terms and correction terms for the spurious collective energy within the cranking approximation [30–45]; all the model parameters have been fitted to essentially all the experimental mass data. While the first HFB-1 mass model [30] aimed at proving that is was possible to
reach a low rms deviation with respect to all experimental masses available at that time, most of the subsequent models were developed to further explore the parameter space widely or to take into account additional constraints. These include in particular a sensitivity study of the mass model accuracy and extrapolation to major changes in the description of the pairing interaction [32,36,39], the spin-orbit coupling [45] or the nuclear matter properties, such as the effective mass [33], the symmetry energy [35,42,43] and the stability of the equation of state [39,42]. The effective interactions correspond either to a standard Skyrme force or to one of its generalized forms including the $t_4$ and $t_5$ terms which are density-dependent generalizations of the $t_1$ and $t_2$ terms, respectively. With such new terms it was possible to reproduce stiff equations of state in infinite neutron matter, as predicted by realistic calculations, and to stop the unphysical transition of neutron matter to a ferromagnetic state at all neutron-proton asymmetries.

With respect to the 2353 measured masses [46], the 29 HFB mass models give an rms deviation ranging between 0.51 MeV for HFB-27 [44] and 0.79 MeV for HFB-1 [30], as illustrated in fig. 3. These rms deviations can be compared to those obtained with other global mass model, such as the Gogny-HFB mass model with the D1M interaction [47] characterised by an rms of 0.79 MeV or the finite-range droplet model (FRDM) [48] with 0.65 MeV. However, when dealing with exotic nuclei far away from stability, deviations between the HFB mass predictions can become significant, not only in the rigidity of the mass parabola, but also in the description of the shell gaps or pairing correlations [49]. The 1σ variance between the 29 HFB mass predictions are illustrated in fig. 4 where deviations around 3 MeV (and up to 5 MeV) can be found at the neutron drip line. Such uncertainties can be interpreted...
as the model uncertainties (due to model defects) [50] and are considered to be independent of parameter uncertainties, but rather a property of the given HFB model. These model uncertainties have been shown to be significantly larger than the uncertainties associated with local variations of the model parameters in the vicinity of an HFB minimum [49], as estimated using a variant of the Backward-Forward Monte Carlo method [51–53] to propagate the uncertainties on the masses of exotic nuclei far away from the experimentally known regions.

Many effective interactions have been proposed to estimate nuclear structure properties within the relativistic or non-relativistic mean-field approach [54]. Except the BSk forces at the origin of the above-mentioned HFB mass models and the D1M interaction at the origin of the Gogny-HFB mass model [47], none of the others have been fitted to a large set of experimental masses. Consequently, their predictions lead to rms deviations typically larger than 2–3 MeV with respect to the bulk of known masses (e.g., masses obtained with the SLy4 force give an rms deviation of the order of 5 MeV [55]). With such a low accuracy, these masses should not be applied to applications, such as the r-process nucleosynthesis. Additionally, other global mass models have been developed, essentially within the macroscopic-microscopic approach [48, 56] but remain unstable with respect to parameter variations, as shown in the framework of the droplet model in ref. [57]. For this reason, more fundamental approaches are needed for practical applications.

When considering mass models obtained in relatively different frameworks, e.g., the Skyrme-HFB or Gogny-HFB mass models, significantly larger deviations are found in the mass predictions away from the experimentally known region. For example, deviations larger than typically 5 MeV are found for exotic neutron-rich nuclei between HFB-21 [42] and D1M [47] mass predictions. However, neutron capture rates may deviate by 3 to 5 orders of magnitude with such mass differences, as illustrated for the Yb isotopes in fig. 2 (upper left panel). Such deviations by far exceed what is acceptable for nucleosynthesis applications. For this reason, further improvements of the mass model is needed. These include development of relativistic as well as non-relativistic mean-field models, but also the inclusion within such approaches of the state-of-the-art corrections, like the quadrupole or octupole correlations by the Generator Coordinate Method and a proper treatment of odd-A and odd-odd nuclei with time-reversal symmetry breaking. Such models should reproduce not only nuclear masses at best, but also as many experimental observables as possible. These include charge radii and neutron skin thicknesses, fission barriers and shape isomers, spectroscopic data such as the $2^+$ energies, moments of inertia, but also infinite (neutron and symmetric) nuclear matter properties obtained from realistic ab initio calculations as well as specific observed or empirical properties of neutron stars, like their maximum mass or mass-radius relations [58].

Future improvements should also take full advantage of the progress made in ab initio calculations in medium mass nuclei. In particular, recently developed methods, such as coupled cluster [59], Dyson or Gorkov self-consistent Greens functions [60, 61], in-medium similarity renormalization group [62] and microscopic shell model [63] are now able to describe nuclear properties in the $15 \lesssim A \lesssim 70$ region successfully, starting solely from the knowledge of the fundamental two- and three-nucleon forces. In a close future, such ab initio calculations should be able to provide tight constraints for mean-field models regarding the binding energies of exotic doubly magic or semi-magic nuclei (see also the contribution of T. Duguet in this Topical Issue).

2.2 Nuclear level densities

NLD are known to play an essential role in reaction theory. Until recently, only classical analytical models of NLD were used for practical applications. In particular, the back-shifted Fermi gas model (BSFG) —or some variant of it— remains the most popular approach to estimate the spin-dependent NLD, particularly in view of its ability to provide a simple analytical formula [64, 65]. However, none of the important shell, pairing and deformation effects are properly accounted for in any analytical description and therefore large uncertainties are expected, especially when extrapolating to very low (a few MeV) or high energies ($U > 15$ MeV) and/or to nuclei far from the valley of $\beta$-stability. Several approximations used to obtain the NLD expressions in an analytical form can be avoided by quantitatively taking into account the discrete structure of the single-particle spectra associated with realistic average potentials. This approach has the advantage of treating in a natural way shell, pairing and deformation effects on all the thermodynamic quantities. Large scale calculations of NLD for nearly 8500 nuclei was performed in the framework of the combinatorial method [66, 67] and has proven its predictive power. One of the main advantages of the combinatorial approach is to provide not only the NLDs tabulated as a function of the excitation energy, but also the spin and parity distributions without any statistical assumption. In particular, it provides naturally non-Gaussian spin distribution as well as...
non-equipartition of parities which are known to have a significant impact on cross section predictions at low energies. Recent developments can now coherently take into account, for deformed nuclei, the transition to sphericity on the basis of a temperature-dependent Hartree-Fock calculation which provides at each temperature the structure properties needed to build the level densities. These combinatorial models have proven their capacity to reproduce experimental data in a satisfactory way, in particular the s- and p-wave resonance spacings, cumulative number of low-lying level, and low-energy total NLD.

The impact of the NLD model on radiative neutron capture rates is illustrated in fig. 2 (upper right panel) where the calculations have been performed either with the HFB plus combinatorial model [66] or the constant temperature (CT) plus Fermi Gas model [65]. Deviations up to a factor of $10^3$ are already found close to the $N = 126$ magic number and up to $10^5$ close to the neutron drip line. This shows how sensitive the neutron capture rates can be with respect to the NLD predictions.

Still several improvements remain to be addressed, such as the treatment of the coupling between particle-hole and vibrational excited states or the control of the smoothing function enabling to suppress the discontinuities between spherical and deformed NLDs [67]. This smoothing function still remains the weakest point of the current formalism. Further investigation are required to be able to suppress such an arbitrary function. Other possible improvements concern the microscopic determination, e.g. within the Quasi-Particle Random Phase Approximation (QRPA), of octupole (and possibly hexadecapole) vibrational levels’ energies for which a phenomenological expression is still employed. The damping of the vibrational enhancement can also be inspired from the results obtained from more microscopic approaches, such as the shell-model Monte Carlo method [68].

### 2.3 Optical potential

Due to the above-mentioned requirements in astrophysics, the phenomenological potential of Woods-Saxon type has long been replaced by the nucleon-nucleus optical potential [69] derived from a Reid’s hard core nucleon-nucleon interaction by applying the Brückner-Hartree-Fock approximation. This so-called JLM potential has been updated by Bauge et al. [70] who empirically renormalized the energy dependence of the potential depth to reproduce scattering and reaction observables for spherical and quasi-spherical nuclei between $^{40}$Ca and $^{209}$Bi in a large energy range from the keV region up to 200 MeV. In this JLMB approach, the renormalization factors are rather well constrained by experimental data, except the low-energy regime of the $\lambda W_1$ factor affecting the isovector imaginary component. The major constraint imposed on the isovector component comes from the quasi-elastic $(p,n)$ scattering data as well as the angle-integrated quasi-elastic $(p,n)$ cross sections to the isobaric analog states at energies above some 20 MeV. For lower energies, the $\lambda W_1$ factor was extrapolated from the confident region around 20 MeV to a constant value of approximately 1.5. Due to the lack of scattering data in the keV region, the low-energy extrapolation of the $\lambda W_1$ factor remained essentially unconstrained. It was recently shown that the isovector contribution to the imaginary component can be adjusted on experimental S-wave neutron strength function data ranging between 1 and 100 keV [71].

To describe the isospin dependence, two cases were studied. The first one (JLMB*) corresponds to a modified value of $\lambda W_1$ at energies below 1 MeV which is larger by 30% with respect to the JLMB value and the second one (JLMB**) by about 50%. These modified potentials have been shown to improve the isospin dependence of the known S-wave neutron strength function of the long Sn and Te isotopic chains [71]. As observed in fig. 2 (lower left panel), for the Yb isotopic chain, the experimental constraints introduced have a drastic impact on the reaction rate. At large neutron excesses, the enhanced $\lambda W_1$ factor strongly reduces the imaginary component, i.e. the neutron absorption channel, and consequently the radiative neutron capture cross section. In particular, it can be seen that, for Yb isotopes with $N \gtrsim 135$, the rates obtained in JLMB* rapidly drop, leading to a totally insignificant resonant neutron capture (for JLMB**, the drop takes place already at $N = 125$). Before drawing any firm conclusion on the neutron capture by exotic neutron-rich nuclei, such a renormalisation of the isovector component of the imaginary potential in the keV region needs to be further constrained by additional theoretical and experimental works.

#### 2.4 $\gamma$-ray strength function

The total photon transmission coefficient from a CN excited state is one of the key ingredients for statistical cross section evaluation. The photon transmission coefficient is most frequently described in the framework of the phenomenological generalized Lorentzian (GLO) model of the giant dipole resonance (GDR) [72,73]. Until recently, this model has even been the only one used for practical applications, and more specifically when global predictions are requested for large sets of nuclei.

The Lorentzian GDR approach suffers, however, from shortcomings of various sorts. On the one hand, it is unable to predict the enhancement of the $E1$ strength at energies below the neutron separation energy demonstrated by different experiments (for a review, see ref. [74]). On the other hand, even if a Lorentzian function provides a suitable representation of the $E1$ strength, the location of its maximum and its width remain to be predicted from some underlying model for each nucleus. For astrophysics applications, these properties have often been obtained from a droplet-type model [75]. This approach clearly lacks reliability when dealing with exotic nuclei, as already demonstrated in refs. [2,76,77].

In view of this situation, combined with the fact that the GDR properties and low-energy resonances may influence substantially the predictions of radiative capture...
cross sections, it is clearly of substantial interest to develop models of the microscopic type which are hoped to provide a reasonable reliability and predictive power for the $E1$-strength function. Attempts in this direction have been conducted within the QRPA model based on a realistic Skyrme or Gogny interactions. In particular, the Skyrme BSk7+QRPA model [78] introduces some phenomenological corrections to take the damping of the collective motion as well as the deformation effects into account. In contrast, the Gogny D1M+QRPA model [79, 80] allows for a consistent description of axially symmetric deformations and includes phenomenologically the impact of multi-particle multi-hole configuration as a function of their densities. Both models have proven their capacity to reproduce experimental photoabsorption data relatively well. QRPA approaches lead to significant departures from a Lorentzian, especially for neutron-rich nuclei, as shown in fig. 5. If qualitatively speaking, the microscopic $E1$ strength functions look rather similar to the phenomenological Lorentzian [64] for nuclei close the valley of $\beta$-stability, major differences are found for exotic neutron-rich nuclei, in particular in the low-energy region where some extra strength, the so-called pygmy resonance, becomes significant in the Skyrme+QRPA predictions [78]. In the Gogny HFB+QRPA calculation, extra-strength is also found in the low-energy tail of the GDR but the strength is more spread than in the Skyrme calculation. Even more strength is found within the relativistic mean field plus QRPA approach, as shown in ref. [81]. The differences illustrated in fig. 5 between analytical and microscopic $\gamma$-ray strength predictions for nuclei far from the valley of stability are also known to have a significant impact on the predicted neutron-capture cross section of astrophysical interest. As shown in fig. 2 (lower right panel), the extra low-lying strength predicted by the QRPA models [78] can give rise to an increase of the neutron capture rate by 1 to 2 orders of magnitude with respect to the classical GLO model [64, 73]. However, QRPA calculations are known to fail reproducing the width (and even the position) of the GDR. To improve the prediction of the $\gamma$-ray strength function, especially at the low energies below the neutron threshold of relevance in radiative neutron captures, it is necessary to go beyond the QRPA scheme by including complex configurations [82] as well as the coupling of single-particle degrees of freedom with the phonon degrees of freedom (the so-called phonon coupling) [83–85]. The low-energy enhancement in the $\gamma$-ray strength function at very low energies (below 1–2 MeV), as derived by the Oslo method [86], may also strongly affect the neutron capture rate close to the neutron drip line, at least if this strength is confirmed to be of $E1$ character [87]. Such a specific property will need to be further investigated, experimentally as well as theoretically. Finally, the M1 excitation mode is still parametrized on the basic of simple Lorentzian-type function and some systematics derived from the little experimental data available [64]. QRPA calculations should also be extended to a global estimate of the $M1$ strength function.

2.5 Direct capture

When the number of available states in the CN is relatively small, the capture reaction is known to be possibly dominated by direct electromagnetic transitions to a bound final state rather than through a compound nucleus intermediary. This DC proceeds via the excitation of only a few degrees of freedom on much shorter time scale reflecting the time taken by the projectile to travel across the target. This mechanism can be satisfactorily described with the perturbative approach known as the potential model [88–92]. It is now well accepted that the DC is important, and often dominant at the very low energies of astrophysical interest for light or exotic nuclei systems for which few, or even no resonant states are available. The direct contribution to the neutron capture rate can be 2 to 3 orders of magnitude larger than the one obtained within the Hauser-Feshbach approach traditionally used in nucleosynthesis applications.
The three CN, pre-equilibrium (PE) and DC reaction mechanisms have been studied systematically and comprehensively within a unique and consistent framework obtained with the modern reaction code TALYS [92–94]. Of particular relevance, the same nuclear inputs are used consistently to determine the three contributions, in particular, the same nucleon-nucleus optical potential ensures that the three components are calculated on the same footing and represents partial fluxes of the same total reaction cross section. Only at temperatures above $T \gtrsim 3 \times 10^4$ K can the PE contribution start to affect the total radiative capture rate [90]. As shown in fig. 6, the DC increases the radiative neutron capture rate by a factor up to $10^4$ for drip line nuclei. Figure 6 shows that most of the neutron-rich regions in between closed neutron shells are dominated by the DC mechanism. However, for some neutron-rich nuclei, no allowed direct transitions may be found (due to selection rules), and the direct channel can consequently be inhibited [95].

Significant uncertainties still affect the DC predictions. These are related to the determination of the nuclear structure ingredients of relevance, i.e. the nuclear mass, spectroscopic factor, neutron-nucleus interaction potential and excited level scheme. A special emphasis needs to be put on the determination of the low-energy excitation spectrum with all details of the spin and parity characteristics. This can be deduced from an NLD model, but within a combinatorial approach, not a statistical one. An important effort needs to be further made to improve the prediction of such nuclear inputs within reliable microscopic models. The transition from the CN to the DC mechanism when only a few resonant states are available also needs to be tackled in a more detailed way, for example within the Breit-Wigner approach.

3 Fission

Since its discovery, fission has always been an active field of research both regarding its purely theoretical challenge and its practical applications. Almost all existing evaluations of the neutron-induced fission cross sections rely on the multiple-humped fission penetration model where barriers are described by inverted decoupled parabolas. Such approaches consider all ingredients as free parameters in order to be able to achieve more or less accurate fits to experimental cross sections [96,97]. Although such adjustments respond to the needs of some nuclear applications, their predictive power remains poor due to the large number of free parameters. Such methods should not be used in applications requiring a purely theoretical description of fission for experimentally unknown nuclei, such as nuclear astrophysics. Recent studies aim at providing sounder descriptions of some of the basic nuclear ingredients required to describe fission cross sections. These concern in particular fission barriers (or more generally fission paths) and NLD at the fission saddle points, but also FFD, including the average number of emitted neutrons. Recently, such nuclear ingredients have been systematically determined in the framework of mean-field models for nuclear astrophysics applications, as described below.

3.1 Fission path

Detailed fission paths have been recently determined on the basis of the Skyrme-HFB model [37] which has proven its capacity to estimate the static fission barrier heights with a relatively high degree of accuracy. The HFB model corresponds to a standard mean-field calculation based on an effective Skyrme interaction. Of particular interest for fission application, the calculation includes all axially symmetric quadrupole, octupole and hexadecapole deformation degrees of freedom, as well as a semi-microscopic quadrupole correlation energy based on the cranking model. Note that such a cranking approximation of the rotational correlation energy has been shown [35] to agree with the exact calculation of Bender et al. [98] and reproduction fairly well experimental moments of inertia. It also includes a high-deformation part for the vibrational correction that is not absorbed into the Skyrme part of interaction, as detailed in ref. [37]. This quadrupole correlation energy has also been shown to be in rather good agreement with the 5-dimensional collective hamiltonian results obtained with the Gogny D1M interaction for all even-even nuclei [42]. The strong deformation dependence of this quadrupole correlation energy turns out to be crucial for a proper description of the nuclear surface at large deformations [37].

The barriers determined within the HFB-14 model [37] reproduce the 52 empirical primary barriers [64] (i.e. the highest barriers of prime interest in cross section calculations) of nuclei with $88 \leq Z \leq 96$ with an rms deviation as low as 0.67 MeV. A similar accuracy is obtained (0.65 MeV) for the secondary barriers. The primary HFB-14 barriers are compared with the empirical ones [64] in fig. 7 where differences up to 1 MeV can be observed. Note that the HFB-14 mass model is also known to reproduce all experimental atomic masses with a high accuracy, namely with an rms deviation of 0.739 MeV with
Fig. 7. (Color online) Deviations between 45 empirical primary fission barriers [64] and those predicted by the HFB-14 [37], FRLDM [100], ETFSI [101], MS99 [102] and HM80 [103] global models for 88 ≤ Z ≤ 96.

Fig. 8. (Color online) Top: Comparison between the HFB-14 and FRLDM primary barriers [100] for even Z isotopic chains relatively close to the valley of stability. Bottom: Same for the HFB-14, ETFSI [101] and MS99 model [102] barriers for Z = 92, 94 and 96 isotopes up to the neutron drip line.

The determination of the fission path is also sensitive to deformation degrees of freedom considered. Global calculations of fission barriers for r-process nuclei assume axial symmetry but allow to break reflection symmetry since the outer barrier is known to be left-right asymmetric. Inner barriers are in many cases also triaxial and only a few calculations take such symmetry breaking into account [105]. Some recent relativistic mean-field studies even show that both non-axial and reflection asymmetric shapes need to be considered simultaneously for the

description of potential energy surfaces and more particularly the outer fission barriers [106]. Such calculations still need to be applied more systematically to the exotic nuclei involved in the r-process.

In comparison with other available compilation of fission barriers, HFB-14 barrier predictions are relatively high, as shown in fig. 8. Already for nuclei close to the stability, the HFB-14 are higher than those predicted by the FRLDM model [100] which drops below 5 MeV for N > 155. For exotic neutron-rich nuclei across the N = 184 shell closure, HFB-14 fission barriers are compared in fig. 8 with the ETFSI and MS99 predictions. HFB-14 barriers show a pronounced shell effect around N = 184, though less than does the ETFSI barriers which are usually higher, except in the N ≃ 170 region. In contrast, the MS99 barriers are by far the lowest with heights between 3 and 5 MeV for the most exotic nuclei. These differences can have a significant impact on fission rate as well as nucleosynthesis predictions [107]. Note that for neutron-rich nuclei with Z ≥ 100 and lying close to the neutron drip line, only HFB-14 barriers are available.
3.2 Fission fragment distribution

The FFD as well as the number of emitted neutrons play a key role in nucleosynthesis simulations since it defines the light species that will be produced by the fission recycling [12,107]. The FFD and A-dependencies of the fragment distribution need to be determined for all potentially fissioning nuclei. Since the widely used Gaussian model of Kodoma and Takahashi [108], a number of new global scission-point models have recently been proposed and extended to exotic nuclei for astrophysical applications. These include in particular the so-called SPY model, corresponding to a renewed statistical scission-point model based on microscopic ingredients [109] and the so-called GEF model estimating the properties of the fission fragments and the emitted neutrons and photons in a global and semi-empirical way [110–112].

Both the SPY and GEF models predict significantly different FFDs, as illustrated in fig. 10 where the yields of eight A = 278 isobars are shown. The FFD of these isobars have a direct imprint on the final r-abundance distribution resulting from NS mergers [12,107]. In the GEF case, the fragment distribution are essentially symmetrical for these particular fissioning nuclei (except for Z = 97–99), whereas a 4-peak distribution is predicted by SPY for all the corresponding isobars. Such doubly asymmetric fragment distributions have never been observed experimentally and can be traced back to the predicted Gogny-HFB potential energies at large deformations for the neutron-rich fragments favored by the A ≃ 278 fission [12]. Detailed Gogny-HFB calculations of the potential energy surface in the parent fissioning nucleus have confirmed qualitatively the presence of these two asymmetric fission modes [12,113].

Finally, we show in fig. 11 the SPY and GEF predictions of the average number of evaporated neutrons for each spontaneously fissioning nucleus. This average number is seen to reach, for both models, values of about four for the A ≃ 278 isobars and maximum values of ∼ 14 for the heaviest Z ≃ 110 nuclei lying at the neutron drip line. This quantity also plays an important role in shaping the final r-process abundance distribution in NS mergers, as shown in refs. [12,107].
the semi-empirical expression HFB calculation at the present time, but approximated by the collective inertial mass which is not estimated from the Of relevance in such calculation is also the calculation of the so-called WKB approximation, as detailed in ref. [99].

fission transmission coefficients are estimated within induced, saddle points to improve our predictions of the neutron-voted to estimate fission paths and NLD at the fission more work within microscopic approaches should be de-

3.3 Perspectives

Fission properties need to be determined on the basis of sound and as microscopic as possible nuclear models. Phenomenological, empirical or systematics extrapolations in the exotic neutron-rich region should be avoided because of their lack of predictive power. Such models could lead to any possible final r-abundance pattern [107]. In contrast, more work within microscopic approaches should be devoted to estimate fission paths and NLD at the fission saddle points to improve our predictions of the neutron-induced, $\beta$-delayed and spontaneous fission rates. So far, the fission transmission coefficients are estimated within the so-called WKB approximation, as detailed in ref. [99]. Of relevance in such calculation is also the calculation of the collective inertial mass which is not estimated from the HFB calculation at the present time, but approximated by the semi-empirical expression $\mu = 0.054 A^{5/3}\text{MeV}^{-1}$ and assumed to be independent of the deformation parameter. Future global calculations should consistently consider the HFB estimates of the inertial mass.

More generally, mean-field model calculations are now available and can be used to estimate the potential energy surfaces and associated collective inertia tensors for a microscopic analysis of the collective dynamics in low-energy fission through a study of the time evolution of the compound system on the basis of a time-dependent Schrödinger equation [113–117]. Such state-of-the-art approach has shown its ability to reproduce several important features of fission, including the fragment kinetic energy and mass distributions [116,117]. Moreover new breakthroughs have recently been achieved [118] to describe low-energy fission up to a few MeV above the fission barrier, where statistical models cannot be applied to treat the excitation energy. This so-called Schrödinger Collective Intrinsic Model may improve the existing microscopic models by taking the particle-vibration couplings into account. Indeed such model is able to describe the couplings of the individuals degrees of freedom to the nucleons collective motion in a fully microscopic and quantum mechanical way, without any other phenomenological parameters than the ones included in the effective nucleon-nucleon interaction.

Similarly, the FFD and the average number of emitted neutrons need to be determined on the basis of sound microscopic models since these ingredients directly influence the calculated abundance distribution. The unexpected doubly asymmetric FFD predicted by SPY also opens new perspectives in theoretical and experimental nuclear physics concerning specific fission modes related to the nuclear structure properties of exotic nuclei. Dynamical mean-field calculations based on the time-dependent generalized coordinate method [114–116] should quantitatively confirm the fission yields predicted by SPY.

4 $\beta$-decay rates

$\beta$-decay rates play a fundamental role in nuclear astrophysics in general [1], and more particularly for the r-process nucleosynthesis since they set the timescale of the nuclear flow and consequently of the production of the heavy elements. $\beta^-$ decays indeed allow high-Z nuclei to be produced from lighter seed nuclei during timescales over which the r-process operates, but also directly influence the relative abundances of product r-nuclides, both locally and globally [107]. Most of the r-process nuclei involved in the r-process have yet to be discovered, so that the use of theoretical models is unavoidable [2]. For a proper prediction of the r-abundances in any r-process site, the $\beta$-decay rates need to be estimated within a factor smaller than typically 1.5.

Only a restricted number of global models of $\beta$-decay rates remains available for nucleosynthesis applications.
These concern the macroscopic Gross Theory (GT2) [119], the FRDM+RPA [120] and the Tamm-Dancoff approximation (TDA) [121]. The deviations between the predictions of these three models are shown in fig. 12 where ratios larger than a factor of 1.5 are found in many neutron-rich regions of the $(N,Z)$ plane. In particular, along the isotonic chains corresponding to closed neutron shells ($N = 50, 82, 126, 184$), responsible for the formation of the r-process peaks observed in the solar system, non-negligible differences can be observed, leading to different estimated r-process peak structures [107].

Here also, more effort needs to be devoted to improve the prediction of $\beta$-decay rates, to include not only the contribution of the forbidden transitions [122, 123] but also the deformation effects, the majority of nuclei being deformed [124]. In particular, the first forbidden transitions have been studied with the finite Fermi system theory [122] and the relativistic QRPA approach [123], but both only for spherical nuclei. Recent studies within the fully self-consistent proton-neutron QRPA model using the finite-range Gogny interaction have now also taken axially symmetric deformations consistently into account [124], but forbidden transition remains to be included. The inclusion of the phonon-phonon coupling has also been shown to give rise to a redistribution of the Gamow-Teller strength and impact the $\beta$-decay half-lives of neutron-rich nuclei significantly [125]. Further progress along all these lines will hopefully help to improve the predictions. Finally, note that on the basis of the $\beta$-decay strength and impact the $\beta$-delayed processes, including neutron emission and fission for the heaviest species, need to be derived. Detailed calculations on the basis of statistical models like TALYS can take full account of the competition of the various open channels (neutron, photon, fission) in the daughter nucleus. Reaction models still need to be better exploited to estimate the probability for such $\beta$-delayed processes.

### 5 Conclusion

Decompressed matter from binary NS mergers remains a viable site for the r-process, which is extremely robust with respect to many astrophysical uncertainties. This robustness, which is compatible with the unique, solar-like abundance pattern of the elements heavier than Ba observed in metal-poor stars, supports the possible creation of these elements by fission recycling in NS merger ejecta. However, the estimated abundance distribution remains rather sensitive to the adopted nuclear models.

A continued effort to improve our predictions of the reaction and $\beta$-decay rates, including their statistical and systematic uncertainties, for nuclei far away from stability is obviously required. The reliability of our predictions today is still far from being at the level of the requirements in nuclear astrophysics applications. Priority should be given to a better description of the ground-state, fission and $\beta$-decay properties, but also NLD, optical potential and $\gamma$-ray strength functions. A huge amount of work is still needed to make full advantage of the development of state-of-the-art microscopic models in building global universal models that include as much as possible the microscopic character of quantum physics. This effort to improve the microscopic nuclear predictions is concomitant with new development aiming at improving the description of the reaction mechanisms, including the equilibrium, pre-equilibrium and direct capture processes. This theoretical work requires simultaneously new measurements of structure properties far away from stability, but also reaction cross sections on stable targets and any experiments that can provide new insight on the numerous ingredients of the reaction models and their extrapolation far away from stability.

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