Eur. Phys. J. A **25**, s01, 653–657 (2005)
DOI: 10.1140/epjad/i2005-06-023-3

EPJ A direct
electronic only

Global microscopic models for r-process calculations

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Received: 15 October 2004 /
Published online: 21 April 2005 –

Abstract. The identification of the astrophysical site and the specific conditions in which r-process nucleosynthesis takes place remain unsolved mysteries of astrophysics. The present paper illustrates the complexity of the r-process nucleosynthesis by describing the nuclear mechanisms taking place during the decompression of neutron star matter, a promising r-process site. Future challenges faced by nuclear physics in this problem are discussed, particularly in the determination of the radiative neutron capture rates by exotic nuclei close to the neutron drip line, as well as the need for improved global microscopic models for a reliable determination of all nuclear properties of relevance.

PACS. 97.10.Cv Stellar structure, interiors, evolution, nucleosynthesis, ages – 32.10.Bi Atomic masses, mass spectra, abundances, and isotopes

1 Introduction

The rapid neutron-capture process, or r-process, is known to be of fundamental importance for explaining the origin of approximately half of the $A > 60$ stable nuclei observed in nature. In recent years nuclear astrophysicists have developed more and more sophisticated r-process models, eagerly trying to add new astrophysical or nuclear physics ingredients to explain the solar system composition in a satisfactory way. 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 discovering astrophysical environments 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 model. However, until now no r-process can be simulated *ab initio* without having to call for an arbitrary modification of the model parameters, leading quite often to physically unrealistic scenarios.

On top of the astrophysics uncertainties, the nuclear physics of relevance for the r-process is far from being under control. The nuclear properties of thousands of nuclei located between the valley of β-stability and the neutron drip line are required. These include the (n, γ) and (γ, n) rates, α- and β-decay half-lives, rates of β-delayed single and multiple neutron emission, and the probabilities of neutron-induced, spontaneous, and β-delayed fission. When considering more complex astrophysics sites like the neutrino-driven wind, proton-, α-, and neutrino-capture rates need to be estimated, too.

New developments of both astrophysics and nuclear physics aspects of the r-process are discussed in this paper. Section 2 describes astrophysics aspects of the r-process nucleosynthesis with a special emphasis on the nucleosynthesis resulting from decompression of initially cold neutron star (NS) matter. It is shown how different the corresponding nuclear mechanisms responsible for the production of r-process elements can be from the more traditional scenarios in core-collapse supernovae. Section 3 is devoted to nuclear physics aspects of the r-process with the description of ground-state and nuclear matter properties within the same framework, and the estimate of the neutron-capture rates by nuclei right at the neutron drip line. Emphasis is made on global microscopic models that have recently been developed to improve the reliability of the extrapolation away from the experimentally known region.

2 Astrophysics aspects of the r-process nucleosynthesis

The origin of the r-process nuclei is still a mystery. One of the underlying difficulties is that the astrophysical site (and consequently the astrophysical conditions) in which the r-process takes place has not been identified. Many scenarios have been proposed. The most favoured sites are all linked to core-collapse supernova or gamma-ray burst explosions. Mass ejection in the so-called neutrino-driven

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wind from a nascent NS or in the prompt explosion of a supernova in the case of a small iron core or an O-Ne-Mg core have been shown to give rise to a successful r-process provided the conditions in the ejecta are favorable with respect to high wind entropies, short expansion timescales or low electron number fractions. Although these scenarios remain promising, especially in view of their significant contribution to the galactic enrichment [1], they remain handicapped by large uncertainties associated mainly with the still incompletely understood mechanism that is responsible for the supernova explosion and the persistent difficulties to obtain suitable r-process conditions in self-consistent dynamical models. In addition, the composition of the ejected matter remains difficult to ascertain due to the remarkable sensitivity of r-process nucleosynthesis to the uncertain properties of the ejecta.

Another candidate site has been proposed as possibly contributing to the galactic enrichment in r-nuclei. It concerns the decompression of initially cold NS matter [2,3,4,5]. In particular, special attention has been paid to NS mergers due to their large neutron densities and the confirmation by hydrodynamic simulations that a non-negligible amount of matter can be ejected [6,7]. Although recent calculations of the galactic chemical evolution [1] tend to rule out NS mergers as the dominant r-process site, it was shown in [5] that this site, or more generally the ejection of initially cold decompressed NS matter in any possible astrophysical scenario, could be one of the most promising r-process sites.

In such a scenario, the nuclear flow towards the production of r-process nuclei is fundamentally different than the one imagined in core-collapse supernovae. The high-density matter constituting the NS inner crust (at typical densities of $\rho \simeq 10^{14}\,\mathrm{g/cm^3}$) is initially at β-equilibrium. The matter composition is characterized by the electron fraction $Y_e = 0.03$ corresponding to a Wigner-Seitz cell made of a $Z = 39$ protons and $N = 157$ neutrons immersed in a neutron sea. As discussed in sect. 3, the initial cell characteristics is sensitive to the effective interaction considered in the nuclear matter equation of state. When the matter starts to expand, the density drop leads to a reduction of the number of neutrons enclosed in the cell, but also to some β-transitions as soon as the respective chemical potentials of neutrons, protons and electrons are such that $\mu_n - \mu_p - \mu_e > 0$ to allow for a neutron to decay into a proton. As the matter reaches the neutron drip line at densities around the drip density of $\rho_{\mathrm{drip}} \simeq 3\cdot 10^{11}\,\mathrm{g/cm^3}$, it is composed of drip nuclei distributed over a relatively large range of elements with $Z = 40$–70 and of free neutrons at a typical density of $N_n \simeq 10^{35}\,\mathrm{cm^{-3}}$. The subsequent decompression leads to a nuclear flow which is closer to the "traditional" r-process, *i.e.* a competition between radiative neutron captures, photodisintegrations, β-decays. In addition, fission processes comes into play as soon as heavy fissioning species are reached. Fission as well as β-decays are also held responsible for a possible increase of the local temperature.

As an example, fig. 1 illustrates the final abundance distribution obtained after the decompression of a clump of material at an initial density $\rho = 10^{14}\,\mathrm{g/cm^3}$. The abundance distribution for $A > 140$ is in relatively good agreement with the solar pattern. In particular the $A = 195$ peak is found at the right place with the right width. It should be stressed that such an r-abundance distribution results from a sequence of nuclear mechanisms that significantly differ from those traditionally invoked to explain the solar r-abundances, namely the establishment of an $(n, \gamma) - (\gamma, n)$ equilibrium followed by the β-decay of the corresponding waiting point. In the present scenario, the neutron density is initially so high that the nuclear flow follows for the first hundreds of ms after reaching the drip density a path touching the neutron drip line. Fission keeps on recycling the material (about 4 times in the example of fig. 1). After a few hundreds of ms, the density has dropped by a few orders of magnitude and the neutron density experiences a dramatic fall-off when neutrons get exhausted by captures. During this period of time, the nuclear flow around the $N = 126$ region follows the isotonic chain. When the neutron density reaches some $N_n = 10^{20}\,\mathrm{cm^{-3}}$, the timescale of neutron capture for the most abundant $N = 126$ nuclei becomes larger than a few seconds, and the nuclear flow is dominated by β-decays back to the stability line.

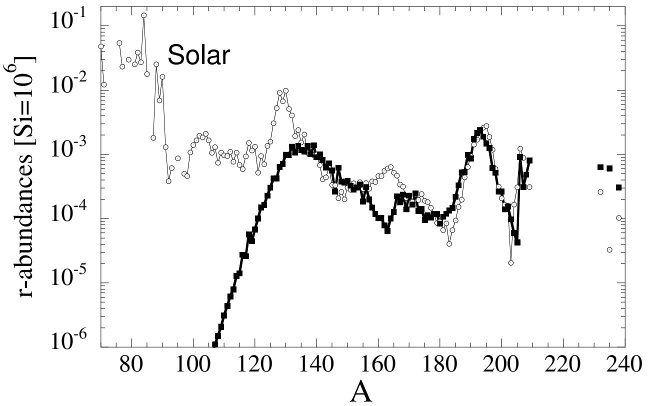

Fig. 1. Final r-abundance distribution for a clump of material at an initial density $\rho = 10^{14}$ g/cm3 (see [5] for more details). The solar system distribution is also shown.

In conclusion, the similarity between the predicted and solar abundance patterns as well as the robustness of the prediction against variations of input parameters make this site one of the most promising that deserves further exploration with respect to various aspects such as nucleosynthesis, hydrodynamics and galactic chemical evolution. More details on the decompression of NS matter can be found in [5] and references therein. This site was described here to illustrate how complex the nuclear mechanisms responsible for the solar r-abundance distribution can be, but also how difficult it remains to ascertain the role of nuclear physics for r-process applications without a clear astrophysics hint about the "real" site. From a nuclear physics point of view, the decompression of NS material is indeed extremely challenging. In addition to the usual requirement for nuclear masses and β-decay rates, as in the traditional scenarios, a detailed knowledge of the radiative neutron capture rates as well as the neutron-induced, spontaneous and β-delayed fission rates is needed for nuclei up to the neutron drip line. Furthemore, the expansion of the high-density NS material needs a detailed description of the nuclear matter equation of state, including its β-decay transition probabilities. Some of these nuclear ingredients are discussed in the next section.

3 Nuclear physics aspects of the r-process nucleosynthesis

Although a great effort has been devoted in recent years to measuring decay half-lives and reaction cross-sections, the r-process involves so many (thousands) unstable exotic nuclei for which so many different properties need to be known that only theoretical predictions can fill the gaps. As illustrated in the previous section, to follow the r-process during the decompression of initially cold NS matter, a detailed knowledge of the various nuclear properties up to and beyond the neutron drip line is required. To fulfill these specific requirements, two major features of nuclear theory must be contemplated, namely its *microscopic* and *universal* aspects. A microscopic description by a physically sound model based on first principles ensures a reliable extrapolation away from the experimentally known region. On the other hand, a universal description of all nuclear properties within one unique framework for all nuclei involved ensures a coherent prediction of all unknown data. A special effort has been made recently to derive all the nuclear ingredients of relevance in reaction theory on the basis of global microscopic models [8]. Some of these issues are discussed now.

3.1 Nuclei and nuclear matter properties

As detailed in [9], a series of Hartree-Fock-Bogolyubov (HFB) mass formulas have recently been constructed. Such HFB calculations are based on a conventional Skyrme force with a density dependent or independent pairing interaction treated in the full Bogolyubov framework with restoration of broken symmetries. A set of 8 mass tables, referred to as HFB-2 to HFB-9, were designed by adjusting the Skyrme force and pairing parameters (the corresponding forces are labeled BSk2 to BSk9, respectively). All mass tables reproduce the full set of 2149 experimental masses [10] with a high level of accuracy, *i.e.* with an r.m.s. error of about 0.65 MeV, except in the case of HFB-9, for which the constraint on a high nuclear-matter symmetry coefficient $J = 30$ MeV raises the r.m.s. value to 0.73 MeV. To test further their predictive power, the HFB calculations were extensively compared to additional observables, namely charge radii and densities, quadrupole moments, giant resonances, nuclear matter properties, (...). As far as the mass extrapolation is concerned, their analysis led to the conclusion that, so far, all these different HFB mass formulas give essentially equivalent predictions, deviations smaller than about 5 MeV being found for more than 8000 nuclei with $8 \le Z \le 110$ lying between the two driplines.

In the context of the r-process nucleosynthesis, it must be stressed that the latest HFB-9 mass table has been designed in order to enable a consistent modelling of the transition from nuclear matter to nuclei, as required in the description of the decompression of initially cold NS matter. More specifically, to conform with realistic calculations of neutron matter at high densities (*e.g.*, [11]), the latest BSk9 force was constrained [9,12] in such a way that the effective isoscalar nucleon mass $M^* = 0.8$, the incompressibility $K_v = 231$ MeV and the symmetry coefficient $J = 30$ MeV. The latter constraint is of particular relevance since it leads to a neutron matter energy per nucleon in excellent agreement with the Friedman and Pandharipande [11] predictions (see [9] for more details). The corresponding Skyrme force is consequently well suited to estimate the initial composition of the NS crust, but also to provide all thermodynamic quantities of relevance during the decompression of the nuclear matter down to densities close to the drip density (below the drip density, the HFB-9 masses provide a consistent description of the nuclear properties). The value adopted for J is of particular importance, especially for a reliable estimate of the initial composition in the NS inner crust. As mentioned above, within the Thomas-Fermi approximation, the β-equilibrated matter at a density of $\rho \simeq 10^{14}$ g/cm^3 is composed of $Z = 39$ and $N = 157$ cells if use is made of the BSk9 force. However, if we consider instead the BSk8 force which is formally equivalent to BSk9 at the exception of being characterized by $J = 28$ MeV, the corresponding cells are typically made of $Z = 82$ protons and $N = 475$ neutrons. The initial conditions for the r-process nucleosynthesis are consequently strongly affected. Future accurate measurements of the neutron-skin thickness of finite nuclei will hopefully help in further constraining the value of J. More details, can be found in [12].

3.2 Nuclear level densities

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. 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 ($U \gtrsim 15$ MeV) and/or to nuclei far from the valley of β-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

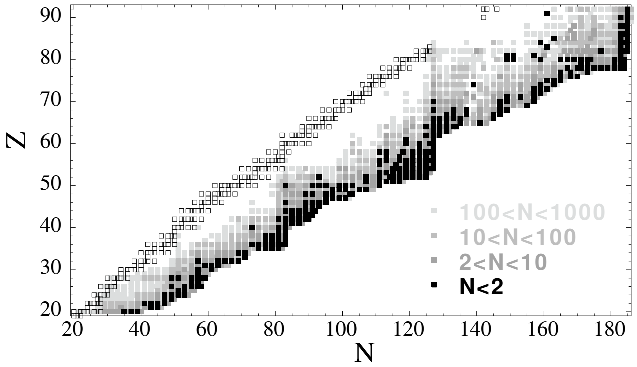

Fig. 2. Representation in the (N, Z)-plane of the total number of levels within a 0.25 MeV energy range above the neutron separation energy. The number of levels is estimated with the HFBCS model of [13]. Only nuclei up to the HFBCS-1 neutron drip line [14] are shown.

all the thermodynamic quantities. The computation of the NLD by this technique corresponds to the exact result that the analytical approximation tries to reproduce, and remains by far the most reliable method for estimating NLD (despite inherent problems related to the choice of the single-particle configuration and pairing strength). The NLD estimated within the statistical approach based on a HFBCS ground-state description was shown [13] to reproduce experimental data (neutron resonance spacings) with the same degree of accuracy as the global BSFG formulas. The HFBCS model provides in a consistent way the single-particle level scheme, pairing strength, as well as the deformation parameter and energy. The HFBCS-based NLD significantly differ from those determined within analytical BSFG-type approaches, even at low energies close to the neutron separation energy.

NLD are not only a fundamental ingredient for the estimate of reaction cross-sections, but also to define somehow the type of reaction mechanisms that are more likely to dominate. So far, all r-process calculations have made use of neutron capture rates evaluated within the Hauser-Feshbach statistical model. Such a model makes the fundamental assumption that the capture process takes place through the intermediary formation of a compound nucleus in thermodynamic equilibrium. The formation of a compound nucleus is usually justified if the level density in the compound nucleus at the projectile incident energy is large enough. However, when dealing with exotic neutron-rich nuclei, the number of available states in the compound system is relatively small and the validity of the Hauser-Feshbach model is questionable. In this case, the neutron capture process might be dominated by direct electromagnetic transitions to a bound final state rather than through the formation of a compound nucleus. To estimate the possible contribution of the direct capture mechanism, fig. 2 gives the total number of levels available in the compound nucleus in an energy range of 0.25 MeV above the neutron separation energy. This interval corresponds to the relevant range of interest for low-energy neutron captures at a typical r-process temperature of about 10^9 K. As seen in fig. 2, many of the nuclei close to the neutron drip line are predicted to have less than 2 levels in the relevant energy range, so that a resonance capture becomes very unlikely. In these conditions, the direct mechanism may dominate. The direct neutron capture rates have been estimated for exotic neutron-rich nuclei [5,15,16] using a modified version of the potential model to avoid the uncertainties affecting the single-particle approach based on the one-neutron particle-hole configuration. Because of the crucial sensitivity of the direct capture cross-section to the spin and parity assignment of the low-energy states in the residual nucleus, only a microscopic combinatorial model of NLD is appropriate. Global calculations within the combinatorial method using the HFB single-particle level scheme and δ-pairing force have now become available [17] and could certainly provide in a near future an accurate and reliable estimate of the intrinsic spin- and parity-dependent level density, and in that respect improve the determination of the resonant as well as direct contributions to the neutron capture by exotic neutron-rich nuclei.

4 γ-ray strength function

The total photon transmission coefficient from a compound nucleus 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 model of the giant dipole resonance (GDR) [16,18]. 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. 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 [19]. This approach clearly lacks reliability when dealing with exotic nuclei.

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 Quasi-Particle Random Phase Approximation (QRPA) model based on a realistic Skyrme interaction. The QRPA $E1$-strength functions obtained within the HFBCS [20] as well as HFB framework [21] have been shown to reproduce satisfactorily the location and width of the GDR and the average resonance capture data at low energies. The aforementioned QRPA

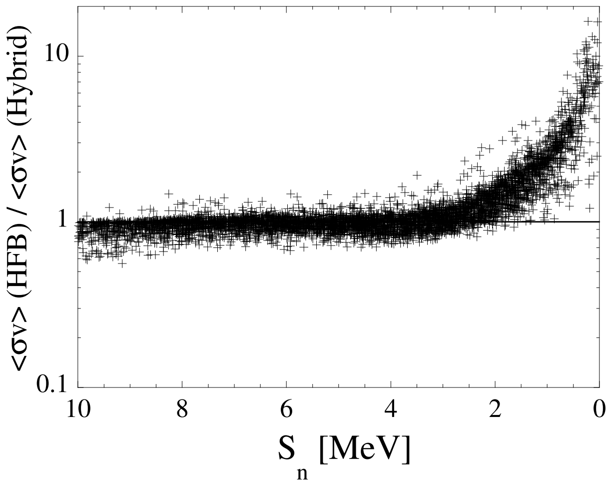

Fig. 3. Ratio of the Maxwellian-averaged (n,γ) rate (at a temperature of 1.5 10^9 K) obtained with the HFB + QRPA $E1$ strength [21] to the one using the Lorentz-type Hybrid formula [16] as a function of the neutron separation energy S_n for all nuclei with $8 \leq Z \leq 110$. The rate is estimated within the Hauser-Feshbach model.

calculations have been extended to all the $8 \leq Z \leq 110$ nuclei lying between the two drip lines. In the neutron-deficient region as well as along the valley of β-stability, the QRPA distributions are very close to a Lorentzian profile. However, significant departures from a Lorentzian are found for neutron-rich nuclei. In particular, QRPA calculations [20,21] show that the neutron excess affects the spreading of the isovector dipole strength, as well as the centroid of the strength function. The energy shift is found to be larger than predicted by the usual $A^{-1/6}$ or $A^{-1/3}$ dependence given by the phenomenological liquid drop approximations [19]. In addition, some extra strength is predicted to be located at sub-GDR energies, and to increase with the neutron excess. Even if it represents only about a few percents of the total $E1$ strength, as shown in fig. 3, it can be responsible for an increase by up to an order of magnitude of the radiative neutorn capture rate by exotic neutron-rich nuclei with respect to the rate obtained with Lorentz-type formulas (for more details, see [20,21]). It should, however, be kept in mind that for such exotic nuclei, as shown in the previous section, the statistical model might not be valid.

5 Conclusions

Most of the problems faced in understanding the origin of r-process elements and observed r-abundances are related to our ignorance of the astrophysical site that is capable of providing the required large neutron flux. In this respect, understanding the r-process nucleosynthesis is essentially an astrophysics issue that will require improved hydrodynamic models to shed light on possible scenarios. Different sites have been proposed, the currently most favoured ones being related to neutrino-driven outflow during supernova or γ-ray burst explosions, but also to the ejection of initially cold decompressed NS matter.

Depending on the astrophysics site, the associated nuclear physics needs can be quite different. At the present time, ignoring the exact r-process site, the only possible strategy is to determine β-decay, neutron-capture, photodisintegration and fission rates for all nuclei which are situated between the valley of β-stability and the neutron drip line. The equation of state of nuclear matter might also play an important role in the determination of the r-process initial conditions. The extrapolation to exotic nuclei constrains the use of nuclear models to the most reliable ones, even if empirical approaches sometime present a better ability to reproduce experimental data. A continued effort is required to improve global microscopic models for a more accurate and reliable description of ground-state properties, nuclear level densities, γ-ray strength functions and optical model potentials (especially for deformed nuclei). This effort is concomitant with new measurements of masses and ground state properties far away from stability, but also reaction cross-sections on stable targets.

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