Shell model studies for nuclear astrophysics

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Abstract. Shell model studies have contributed in recent years significantly to improve nuclear input required in simulations of the dynamics of astrophysical objects and their associated nucleosynthesis. This manuscript highlights a few examples like electron capture rates of importance for the evolution of core-collapse supernovae and the nucleosynthesis in thermonuclear supernovae, neutrino-nucleus cross sections with relevance to the supernova neutrino spectra and finally half lives of neutron-rich nuclei with magic neutron numbers which serve as waiting points in the mass flow of the astrophysical r-process.

1. Introduction

The advances of computer hardware, decisive progress in modelling and the development of powerful computer codes has strengthened the position of the interacting shell model as the method of choice to describe medium-mass nuclei [1, 2]. Such nuclei play often crucial roles for the dynamics of astrophysical objects and their associated nucleosynthesis. However, a direct experimental determination of the required input is often prohibited due to the extreme conditions of the astrophysical environment and hence the information has to be modelled. Here the shell model has become the method of choice due its ability to account for the relevant correlations among nucleons and to accurately reproduce low-energy spectra and electromagnetic transitions [3, 4].

This manuscript will highlight a few examples where shell model studies, exploiting the diagonalization and Shell Model Monte Carlo (SMMC) varieties of the approach, have contributed to a better understanding of astrophysical objects. Diagonalization shell model calculations have been performed to derive rates for weak interaction processes of nuclei up to the iron-nickel mass range [5, 6, 7]. In particular, the shell model rates for electron captures on nuclei have significant impact on the presupernova core evolution of massive stars [8, 9] and on the nucleosynthesis in thermonuclear supernovae [10]. For r-process nucleosynthesis shell model calculations of half lives for neutron-rich nuclei with magic neutron numbers (called waiting points) indicate that the r-process mass flow through these waiting points is faster than previously anticipated [11, 12, 13]. The SMMC approach allows to derive nuclear properties at finite temperature in extremely large model spaces taking the relevant nuclear correlations into account [14, 15]. The SMMC has been the base to derive electron capture rates for heavier neutron-rich nuclei for which cross-shell correlations are essential establishing capture on nuclei as the main weak interaction process for the dynamics of the core collapse of a massive star [16, 17, 18]. The SMMC also allows for the microscopic derivation of nuclear level densities

[19, 20] which is an important input for calculations of nuclear reaction rates in the framework of the statistical model. Such calculations are reviewed by Yoram Alhassid in this volume.

2. Electron captures in supernovae

A massive star ends its life in a supernova explosion triggered by the gravitational collapse of its inner core which is no longer supported by energy released in charged-particle reactions [21, 18]. Electron captures on nuclei have three important consequences during the collapse [22, 3]: i) they reduce the number of electrons and hence the pressure which the degenerate (relativistic) electron gas can stem against the gravitational contraction; ii) the neutrinos, generated by the capture process, leave the star mainly unhindered carrying away energy and keeping the entropy in the core low such that heavy nuclei survive during collapse, iii) electron capture changes a proton in the nucleus into a neutron driving the core composition to more neutron-rich (and heavier) nuclei.

At the stellar conditions, at which the core composition (described by Nuclear Statistical Equilibrium) is dominated by nuclei from the iron-nickel mass range (pf shell nuclei), the capture process is dominated by GT_+ transitions[1]. Thanks to advances in computer hardware and in nuclear modelling it has become possible to study the low-energy spectra and transitions of pf-shell nuclei in the respective model space [1]. In fact it turned out that, besides a constant renormalization of the Gamow-Teller operator [23, 24], such highly correlated wave functions are required to describe the strong fragmentation and total value of the GT_+ strength [25] as experimentally determined by charge-exchange experiments. The pioneering work to measure GT_+ strength functions has been performed at TRIUMF using (n,p) reactions, achieving, however, only modest energy resolutions [26]. This situation has been dramatically improved by the development of the (d,^{2}He) technique at the KVI Groningen which allowed to determine GT_+ distributions for many nuclei in the iron-nickel mass range with an energy resolution of about 150 keV [27].

We note that the strong energy dependence of phase space as well as the fact that the electron Fermi energy is of the same order as the Q-value of the abundant nuclei under presupernova conditions, makes a detailed and accurate description of the GT_+ distribution an important requirement for a reliable description of stellar electron capture during this phase of the collapse. That the diagonalization shell model is up to this task and indeed the method of choice to describe stellar weak-interaction rates during presupernova collapse has been recently demonstrated by Cole and collaborators [28]. These authors compared capture rates derived from experimental GT_+ data for all pf shell nuclei, for which data exist, with rates calculated within the shell model using two different residual interactions. As is shown in Fig. 1 the agreement is quite satisfactory at the conditions at which these nuclei are abundant and relevant for the core dynamics (right panel).

We note that in the stellar environment electron capture is reduced (approximately by a factor of order 2) due to screening effects [31]. As beta decays are enhanced by screening, stellar environment effects can alter the conditions at which URCA pairs operate. This is particularly important for the core collapse of $8-12M_\odot$ stars, (electron capture supernovae) [32], where several URCA pairs influence the dynamics of the core evolution. Stars in this mass range develop degenerate ONe or ONeMg cores which are driven towards collapse by the loss of electron pressure support due to electron captures, mainly in the very abundant nuclear species ^{20}Ne and ^{24}Mg [32, 33]. Ref. [7] has evaluated the electron capture rates on ^{20}Ne, ^{20}F, ^{24}Mg, ^{24}Na and the β decay rates for ^{20}Na and ^{24}Na at temperature and density conditions relevant

[1] The subscript refers to the isospin component in the GT operator such that in GT_+ transitions a proton is changed into a neutron, in GT_- transitions, relevant for β decay of nuclei with neutron excess, a neutron is changed into a proton, and the GT_0 strength, important to describe low-energy inelastic neutrino-nucleus scattering, refers to transitions between proton states and neutron states, respectively

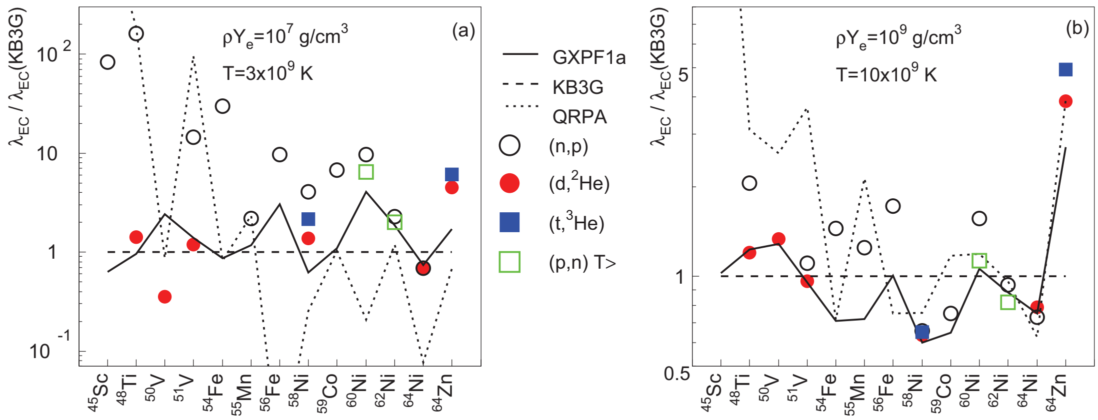

Figure 1. Comparison of electron captures rates as function of temperature calculated from experimental GT_+ data and distributions calculated within the large-scale shell model with two different interactions (KB3G [29] and GXPF1 [30]) and within the QRPA approach. The left and right panels correspond to conditions during the earlier stages of the collapse where the capture rates are sensitive to details of the GT_+ distribution. (from [28]).

for the late-evolution stages of stars with $M = 8 - 12 M_\odot$, based on recent experimental data and large-scale shell model calculations.

In the later stage of the collapse of massive stars, the nuclei present in the core composition get heavier and more neutron-rich. The appropriate model space to describe electron capture for such nuclei is too large (requiring two major shells) to allow for shell model diagonalization calculations. The calculations are then based on a statistical shell model approach (Shell Model Monte Carlo [15]) which allows to determine nuclear properties at finite temperature and in large multi-shell model spaces taking the relevant nuclear correlations into account. Such correlations are particularly important for nuclei with proton number below and neutron number above an oscillator shell closure (like N=40). In such situations GT_+ transitions would be completely blocked by the Pauli principle in the Independent Particle Model (IPM) [34] suppressing electron capture on nuclei drastically. However, it has been shown in [16] that nuclear correlations induced by the residual interaction move nucleons across the shell gap enabling GT_+ transitions and making electron capture on nuclei the dominating weak interaction process during collapse [16, 46]. We add two remarks: The unblocking of the GT_+ strength across the $N = 40$ shell closure has been experimentally confirmed for ^{76}Se (with 34 protons and 42 neutrons) [35], in agreement with shell model studies [37]. Supplemented by transfer reaction experiments [36] the shell model study shows that the neutron occupation numbers in the $g_{9/2}$ orbital is about 6 (rather than 2 as in the IPM). Furthermore, shell model studies clearly show that the description of cross-shell correlations is a rather slowly converging process requiring the consideration of multi particle-multi hole configurations [38, 39, 37]. The diagonalization shell model electron capture rates agree reasonably well with those obtained by the SMMC+RPA approach at such astrophysical conditions at which nuclei with $Z < 40, N > 40$ dominate.

The modern shell model weak-interaction rates have significant impact on collapse simulations. In the presupernova phase ($\rho < 10^{10}$ g/cm^3) the captures proceed slower than assumed before and for a short period during silicon burning β-decays can compete [8, 9]. As a consequence, the core is cooler, more massive and less neutron rich before the final collapse. However, until recently simulations of this final collapse assumed that electron captures on nuclei are prohibited by the Pauli blocking mechanism, mentioned above (e.g. [21]). However, based on the SMMC calculations it has been shown in [16] that capture on nuclei dominates over capture on free protons. The changes compared to the previous simulations are significant [16, 17, 18]. Importantly the shock is now created at a smaller radius with more infalling material to traverse, but also the density, temperature and entropy profiles are strongly modified [17].

Finally we note that the shell model electron capture rates [6, 42], which are noticeably slower than the pioneering rates of Fuller *et al.* (FFN) for pf shell nuclei [40], have important consequences in nucleosynthesis studies for thermonuclear (type Ia) supernovae by less reducing the electron-to-nucleon ratio behing the burning front [10]. As a consequence very neutron-rich nuclei like ^{50}Ti and ^{54}Cr are significantly suppressed compared to calculations which use the FFN rates [41]. In fact, in calculations using the shell-model rates no nuclide is significantly overproduced compared to solar abundances [10].

3. Neutrino-nucleus scattering

The shell model has also been used to derive inelastic neutrino-nucleus cross sections for applications in supernova dynamics and nucleosynthesis. To validate this approach it has been exploited that the GT_0 strength, which is relevant for neutrino scattering on nuclei at supernova neutrino energies, is, in a very good approximation, proportional to the M1 strength of spherical nuclei [43]. Precision M1 data, obtained by inelastic electron scattering for such nuclei, are well reproduced by shell model calculations, which are also used to derive GT_0 distributions for excited nuclear states which can be thermally populated at finite supernova conditions [43, 44]. At higher neutrino energies forbidden transitions can contribute to the inelastic scattering cross section which have been derived by RPA calculations. Supernova simulations which incorporate inelastic neutrino-nucleus scattering indicate that this mode has a noticeable effect on the early neutrino spectra emitted from supernova [45]. Here nuclei act as obstacles to high-energy neutrinos which are down scattered in energy. This reduces significantly the tail of the neutrino spectra and hence also the predicted event rates for the observation of supernova neutrinos by earthbound detectors [45]. The simulations also show that inelastic neutrino-nucleus scattering contributes only slightly to the neutrino thermalization with matter during the collapse [18]. Recent studies also indicate that nuclear deexcitation by neutrino pair emission has no impact on the collapse dynamics [46]. It is, however, the dominating source of $\bar{\nu}_e$ and ν_μ, ν_τ neutrinos during collapse.

4. Half-lives of r-process waiting points

The r-process is the astrophysical origin of about half of the elements heavier than iron. It occurs in an astrophysical environment with extreme neutron densities [47], associated with neutron star mergers [48] and the neutrino-driven wind in a core-collapse supernova [49]. The r-process path in the nuclear chart runs through nuclei with such large neutron excesses that most of them have yet not been made in the laboratory and their properties have to be modelled. Of particular importance are the nuclei with magic neutron numbers. With their relatively long half-lives they act as obstacles in the r-process flow (so-called waiting points).

There have been a few crucial half-life measurements of waiting points with $N = 50$ and 82. These data turned out to be shorter than anticipated by global predictions based on QRPA models, likely pointing to the importance of correlations beyond such approaches. Such correlations have been considered in shell model studies performed for the waiting point nuclei. These studies, in some cases done before the measurement, achieved in general good agreement with the experimental half lives [11, 3]. Very recently the shell model calculations have been extended to include also contributions from forbidden transitions [12, 13] which turn out to reduce the half lives for the $N = 126$ waiting points significantly. This fact had already been noticed previously by Borzov [50]. By using recent half-life data for neutron-rich nuclei he also succeeded to improve the Fayan's density functional to achieve a rather accurate description of measured half lives [50] (see Fig. 2). Unfortunately Borzov's approach is currently limited

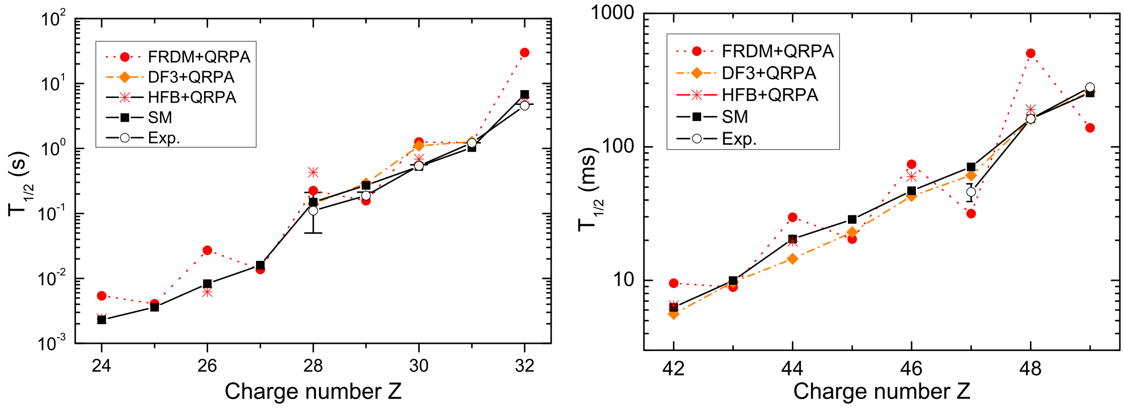

Figure 2. Comparison of shell model half lives for $N = 50$ (left) and $N = 82$ r-process waiting point nuclei with data and predictions from other models (from [13]).

to spherical nuclei, while the shell model studies are even more restricted to nuclei with magic neutron numbers. Nevertheless these calculations, together with the available data, indicate that the mass flow in the r-process to heavier nuclei is faster than anticipated from previous simulations. This can have interesting consequences for the competition of beta decays and neutron captures at freeze out [51]. In particular for r-process simulations within the neutron star merger scenario the faster half lives can lead to faster fission cycling influencing the supply of free neutrons after freeze out [52, 53]. Fission cycling is a characteristic of r-process simulations for neutron star mergers. Here the very extreme neutron densities support mass flow up to the mass range $A \sim 280 - 300$ where the nuclei decay by fission, producing nuclides around ^{132}Sn as fission fragments. Simulations thus have the interesting feature that the third peak is generated by neutron captures already before freeze-out, while the second peak at $A \sim 130$ and the lead peak develop as products of fission and alpha decays, respectively, at late stages of the process after freeze out. While the r-process abundance pattern depends somewhat on the fission yield distributions, it is relatively insensitive to the underlying neutron star models [48] and the adopted nuclear mass models [54]. Hence the neutron star merger scenario with its characteristic fission cycling might be able to describe the rather robust pattern of r-process abundances between the second and third peaks as it is observed in old stars [55].

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