CALCULATIONS OF NUCLEAR REACTIONS OF ASTROPHYSICAL INTEREST INVOLVING UNSTABLE NUCLEI

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Abstract: Nuclear reactions involving unstable nuclei play an important role in nucleosynthesis. Such reactions are mainly associated with explosive astrophysical scenarios occurring at the final stages of stellar evolution. For many nuclear reactions involving unstable nuclei the direct reaction mechanism cannot be neglected and may even be the dominant reaction mechanism. For example, the direct–reaction mechanism can be important for neutron capture by neutron–rich nuclei. We investigate the role of the direct–reaction mechanism for the two reactions ^{36}S(n,γ)^{37}S and ^{124}Sn(n,γ)^{125}Sn on the neutron–rich border of the region of stability.

Nuclear–structure models are indispensable for extrapolating reaction rates to nuclei near and far–off the region of stability. The above two reactions are considered as benchmarks for different nuclear–structure models (Shell Model, Relativistic Mean Field Theory, Quasi Particle Random Phase Approximation, Hartree Fock Bogoliubov Theory).

1 Introduction

All chemical elements and their isotopes found in the Universe are produced by nuclear reactions in various astrophysical sites. Stellar nucleosynthesis plays a crucial role in the evolution of stars and is one of the stringent tests of stellar models. In the last decades investigations concentrated mainly on stellar nuclear reactions between stable nuclei occurring in quiescent phases of stellar evolution and taking place at relatively low temperature sites. New challenges for nuclear physics and astrophysics are, without doubt, the various astrophysical events in hot and especially in explosive scenarios and the concomitant nucleosynthesis involving nuclear reactions with radioactive nuclei. The interaction of such highly unstable nuclei with nucleons and α–particles, as well as other nuclei, has lent itself only partially to direct experimental measurements, so that the determination of the reaction rates relies heavily on theoretical models. This requires powerful theoretical nuclear–structure methods, since there are severe limitations to the experimental determination of input parameters for the calculation of reaction and decay rates. Only if the half–lives are of the order of 1 s or longer, the cross sections of nuclear reactions can be measured by using radioactive ion beams (for nuclei with half–lives $t_{1/2} \approx 1\,\mathrm{s} - 1\,\mathrm{h}$) or radioactive targets (for nuclei with half–lives $t_{1/2} \gtrsim 1\,\mathrm{h}$). For nuclei far–off stability often experimental data is not available at all.

Supernovae of type II could provide the conditions required for the so–called α– and r–processes. The α–process occurs in the neutrino–heated hot bubble between the nascent neutron star and the overlying stellar mantle of a type–II supernova [1−5]. During the gravitational collapse in the supernova the temperature in the core of the star gets so high (up to 10^{10} K) that all the nuclei are disassembled into protons and neutrons by photodissociation. Afterwards, the material, initially having been in nuclear statistical equilibrium (NSE) at high temperature, is expanded and cooled so rapidly that not all the α–particles have time to reassemble. In this environment most nucleons are either in the form of free neutrons or bound in α–particles.

The nucleosynthesis in the neutrino bubble takes place in subsequent steps: first, in this scenario α–particles are formed from the free nucleons. Then, in the following α–process, nuclei up to about $A \approx 100$ are produced [1]. Here the main nuclear processes are neutron–induced capture reactions as well as β^-–decays, even so proton–induced transfer reactions and α–induced reactions are also relevant. Finally, the neutrino bubble is also an ideal site for the r–process synthesizing the elements of about $A \geq 100$ [1,6,7]. In the r–process, neutron capture on neutron–rich targets far–off stability is practically the only existing reaction type, and is competing with β^-–decay. For these reactions the direct reaction mechanism is not negligible and even is the dominating mechanism in many cases.

In Section 2 the direct reaction mechanism is discussed and applied to the two reactions ^{36}S(n,γ)^{37}S and ^{124}Sn(n,γ)^{125}Sn. Finally, in Section 3 the above reactions will be investigated as benchmarks for the applicability of different nuclear–structure models (Shell Model, Relativistic Mean Field Theory, Quasi Particle Random Phase Approximation, Hartree Fock Bogoliubov Theory) in calculating cross sections at the border and far–off the region of stability.

2 Direct capture

In astrophysically relevant nuclear reactions two opposite reaction mechanisms are of importance, compound–nucleus formation and direct reactions. At the low reaction energies occurring in primordial and stellar nucleosynthesis the direct mechanism often cannot be neglected and can even be dominant. The reason for this behavior is that only a few levels exist for low excitations of the compound nucleus. For instance, this is the case for neutron capture by neutron–rich nuclei. The importance and even dominance of direct capture has already been demonstrated for magic nuclei and at the border of the region of stability (see e.g. [8]) for neutron capture by neutron–rich nuclei).

The Direct Capture (DC) cross section for a reaction $A(a,\gamma)B$ is given by [9,10]):

$$\sigma_{DC} = 2\left(\frac{e^2}{\hbar c}\right)\left(\frac{\mu c^2}{\hbar c}\right)\left(\frac{k_\gamma}{k_a}\right)^3 \frac{1}{2I_A+1}\,\frac{1}{2S_a+1}\int d\Omega \sum_{M_A M_a M_B,\sigma} |T_{M_A M_a M_B,\sigma}|^2 \quad . \tag{1}$$

The complete DC formalism can also be found in [11]). The computer code TEDCA [12]) was used to calculate the DC cross sections.

The quantities I_A, I_B and $S_a (M_A, M_B$ and $M_a)$ are the spins (magnetic quantum numbers) of the target nucleus A, residual nucleus B, and projectile a, respectively. The reduced mass in the entrance channel is given by μ. The polarization σ of the electromagnetic radiation can be ± 1. The wave numbers in the entrance channel and for the emitted radiation are denoted by k_a and k_γ.

For the analysis of the reactions in this work we have only taken into account the electric dipole transition: $T = T^{E1}$. This transition amplitude depends on the overlap integrals of the bound–state wave function $u_{NLJ}(r)$, the scattering wave function $\chi_{l_a j_a}$, and the transition operator $\mathcal{O}^{E1}$

$$I^{E1}_{l_a j_a} \sim C(E1)\int dr\, u_{NLJ}(r)\,\mathcal{O}^{E1}(r)\,\chi_{l_a j_a}(r) \quad . \tag{2}$$

with

$$C(E1) \;=\; i\mu\left(\frac{Z_a}{m_a} - \frac{Z_A}{m_A}\right) \quad . \tag{3}$$

The theoretical capture cross section σ^{th} is usually obtained by multiplying the DC cross section σ^{DC} with the isospin Clebsch–Gordan coefficient C and the spectroscopic factor S of the final state: $\sigma^{th} = C^2 S \cdot \sigma^{DC}$.

In Table 1 the results of the DC–calculations for ^{36}S(n,γ)^{37}S are compared with experimental data. Details of the experimental measurements and the DC–calculations for this reaction are given elsewhere [13]). All the relevant input parameters for the DC–calculations were taken from experimental data (see Table 1). The cross sections calculated in DC excellently reproduce the experimental data for ^{36}S(n,γ)^{37}S, showing that DC is the dominating reaction mechanism in this case. The only discrepancy occurs for a projectile energy of 198 keV, where resonant CN–contributions should also be taken into account in the theoretical calculations.

Table 1: Final states, Q–values, transitions and spectroscopic factors for the states of ^{37}S obtained from ^{36}S(d,p)^{37}S [14]. Cross sections of ^{36}S(n,γ)^{37}S at 25.3 meV, 25 keV, 154 keV, 198 keV and 225 keV using direct capture are compared with the experimental data.

Final state	Q–value[1] [MeV]	Transition	Spectroscopic factor	Cross section 25.3 meV [mbarn]	25 keV [μbarn]	155 keV [μbarn]	198 keV [μbarn]	224 keV [μbarn]
$\frac{7}{2}^-$	4.303	d $\rightarrow$ f	0.50	0.0	0.0	0.1	0.2	0.2
$\frac{3}{2}^-$	3.657	s $\rightarrow$ p	0.55	157.1	158.0	63.6	56.5	53.3
$\frac{3}{2}^+$	2.906	p $\rightarrow$ d	0.03	0.0	0.0	0.0	0.0	0.0
$\frac{3}{2}^-$	2.312	s $\rightarrow$ p	0.03	5.3	5.3	2.2	1.9	1.8
$\frac{1}{2}^-$	1.666	s $\rightarrow$ p	0.47	28.3	28.5	11.5	10.3	9.8
Total cross section: DC				190.7	191.8	77.4	68.9	65.1
Total cross section: experiment				150 ± 30[2]	187 ± 14	80 ± 7	121 ± 11	77 ± 7

[1] Refs. [15,16]

[2] Ref. [17]

We also calculated the DC cross section for ^{124}Sn(n,γ)^{125}Sn using the experimentally available excitation energies of ^{125}Sn and spectroscopic factors extracted from ^{124}Sn(d,p)^{125}Sn [19] and ^{124}Sn(α,τ)^{125}Sn [20] (Table 2). The situation is somewhat different in this case as compared to ^{36}S(n,γ)^{37}S. The level density of the compound nucleus ^{125}Sn at the neutron threshold is much higher than for ^{37}S. With a recent level–density formula including microscopic corrections and thermal damping of shell effects [21] we found the values 6.8/MeV and 1247/MeV for the level density at the neutron separation energy for ^{37}S and for ^{125}Sn, respectively. No experimental information is available for thermonuclear projectile energies in ^{124}Sn(n,γ)^{125}Sn. For this reaction, we could only make a comparison of the DC calculation with experiment only at thermal energies, because no cross–section data was available at thermonuclear energies. Using DC for the thermal cross section we obtain a cross section value of 39.3 mb, as compared to the experimental value (133 ± 5) mb. Despite the high level density the DC contribution to the cross section is still about 30%. However, in more neutron–rich isotopes the excitation energy of the compound nucleus gets lower, also leading to a substantial diminution of the level density of the compound nucleus. Thus, the DC–contribution becomes the dominating reaction mechanism.

3 Benchmarks of nuclear–structure models

In this section, DC–calculations of ^{36}S(n,γ)^{37}S and ^{124}Sn(n,γ)^{125}Sn will be used as benchmarks for the applicability of different nuclear–structure models (Shell Model: SM, Relativistic Mean Field Theory: RMFT, Quasi Particle Random Phase Approximation: QRPA, Hartree Fock Bogoliubov Theory: HFB) in extrapolating cross sections from the border of the region of stability to the drip line. Such extrapolations are necessary for the determination of cross

Table 2: Excitation energies ^{125}Sn [18], Q–values for transitions to ^{125}Sn [18] and spectroscopic factors extracted from ^{124}Sn(d,p)^{125}Sn [19] and ^{124}Sn(α,τ)^{125}Sn [20] used in the calculation of the direct contribution of ^{124}Sn(n,γ)^{125}Sn

J^π	E_{exc} [MeV]	Q [MeV]	Spectroscopic factor
$\frac{11}{2}^-$	0.000	5.733	0.41
$\frac{3}{2}^+$	0.028	5.705	0.44
$\frac{1}{2}^+$	0.215	5.578	0.33
$\frac{7}{2}^-$	2.767	2.966	0.54
$\frac{3}{2}^-$	3.349	2.384	0.14
$\frac{3}{2}^-$	3.421	2.311	0.36
$\frac{3}{2}^-$	3.830	1.903	0.10
$\frac{3}{2}^-$	4.060	1.673	0.14

Table 3: Spectroscopic factors of ^{37}S obtained from different nuclear–structure models (SM, RMFT, QRPA, HFB) and from one–nucleon transfer (EXP)

J^π	SM	RMFT	QRPA	HFB	EXP
$\frac{7}{2}^-$	0.91	0.824	0.988	0.835	0.50
$\frac{3}{2}^-$	0.86	0.922	0.995	0.998	0.55
$\frac{3}{2}^+$	–	–	–	–	0.03
$\frac{3}{2}^-$	–	–	–	–	0.03
$\frac{1}{2}^-$	0.97	0.972	–	–	0.47

sections for neutron capture in the α– and r–process.

For all the nuclear structure models considered in the following we assumed spherical symmetry for ^{37}S and ^{125}Sn. The SM input was taken from calculations in the combined psd–shell with an effective nucleon–nucleon interaction derived by Wildenthal [22]. The RMFT input was determined from calculations using the parameter set NL1 [23]. The HFB input was obtained using the SkP variant of the Skyrme interaction developed in [24]. The QRPA input was extracted from a single–particle model using folded Yukawa single–particle potentials [25].

To be able to make a meaningful comparison we used the same experimentally determined nuclear masses [15] and the same folding potentials in the entrance and exit channels [13,26] for all calculations of the capture cross sections. However, the excitation energies and spectroscopic factors were extracted from experimental data as well as from the different nuclear–structure models given above.

Figure 1: Excitation energies of ^{37}S from experimental data (EXP), Shell Model (SM), Quasi Particle Random Phase Approximation (QRPA), Relativistic Mean Field Theory (RMFT) and Hartree Fock Bogoliubov Theory (HFB)

3.1 Results for ^{36}S(n,γ)^{37}S

The excitation energies for ^{37}S, obtained from experiment and from the different models (SM, RMFT, QRPA, HFB), are shown in Fig. 1. The corresponding spectroscopic factors for the transitions to the different final states for ^{37}S are given in Table 3.

The results of the DC cross sections, with the input parameters taken from the theoretical models and experimental data, for ^{36}S(n,γ)^{37}S at 25 keV are compared in Table 4. It should be noted that if the input data (excitation energies and the spectroscopic factors) of the DC calculation for the cross section are taken from experimental data, excellent agreement with the experimental cross section is obtained (Table 1). This DC–calculation for ^{36}S(n,γ)^{37}S at 25 keV (sixth column of Table 1 or last column in Table 4) is in the following compared with DC–calculations with the input taken from the different nuclear structure models.

The results using the different nuclear–structure models vary between about one third

Figure 2: Excitation energies of ^{37}S from experimental data (EXP), Relativistic Mean Field Theory (RMFT), Quasi Particle Random Phase Approximation (QRPA) and Hartree Fock Bogoliubov Theory (HFB)

(QRPA) and almost twice (SM) of the experimental cross section. This discrepancy has two reasons:

(i) All nuclear structure models (SM, RMFT, QRPA, HFB) yield spectroscopic factors that are about 50–100% higher than the ones extracted from one–nucleon transfer (EXP) (Table 2). This leads to an enhancement of the DC–cross section by the same factor.

(ii) The dominating transitions are the ones to the final states $3/2^-$ and $1/2^-$ in ^{37}S, because only for these transitions an E1–transition from an incident s–wave is possible. For all other final states either the higher multipole order or/and the centrifugal barrier in the entrance channel suppresses the transition. In all our nuclear structure models except SM the relevant $3/2^-$– and $1/2^-$–states have a higher excitation energy. In QRPA and HFB the $1/2^-$–state is not even bound at all.

Therefore, due to the larger spectroscopic factors the DC–calculation using the SM–input is enhanced by about 50%, whereas for RMFT the higher spectroscopic factor is almost canceled

Table 4: Comparison of the DC cross section for ^{36}S(n,γ)^{37}S at 25 keV in μbarn with the input from the different structure models (SM, RMFT, QRPA, HFB) and the input determined from experimental data (EXP)

J^π	SM	RMFT	QRPA	HFB	EXP
$\frac{7}{2}^-$	0.016	0.014	0.017	0.015	0.009
$\frac{3}{2}^-$	243.896	211.749	61.531	90.534	157.988
$\frac{3}{2}^+$	–	–	–	–	0.007
$\frac{3}{2}^-$	–	–	–	–	5.264
$\frac{1}{2}^-$	70.092	18.079	–	–	28.520
$\sum \sigma_{DC}$:	314.004	229.842	61.548	90.549	191.787

Table 5: Spectroscopic factors of ^{125}Sn obtained from nuclear–structure models (RMFT, HFB, QRPA) and from one–nucleon transfer (EXP)

J^π	RMFT	HFB	QRPA	EXP
$\frac{11}{2}^-$	0.484	0.481	0.775	0.41
$\frac{3}{2}^+$	–	–	–	0.44
$\frac{1}{2}^+$	–	–	–	0.33
$\frac{7}{2}^-$	0.985	0.982	0.998	0.54
$\frac{3}{2}^-$	–	–	–	0.14
$\frac{3}{2}^-$	–	–	–	0.36
$\frac{3}{2}^-$	–	–	–	0.10
$\frac{3}{2}^-$	–	–	–	0.14

out by the lower Q–value in the calculation of the DC cross section. For the other two models, there is no contribution from the transition to the $1/2^-$–state, and the Q–value for the transition to the $3/2^-$–state is much lower, so that in this case the DC–cross section is only about 1/2 (HFB) and 1/3 (QRPA) of the experimental value.

3.2 Results for ^{124}Sn(n,γ)^{125}Sn

The excitation energies obtained from experiment and from the different nuclear–structure models (RMFT, HFB, QRPA) for ^{125}Sn are shown in Fig. 2. In this case no shell–model results are available. The corresponding spectroscopic factors for the transitions to the respective final states for ^{125}Sn are given in Table 5.

The results of the DC cross sections with the input parameters taken from the different structure models (RMFT, HFB, QRPA) and from one–nucleon transfers (EXP) are compared for ^{124}Sn(n,γ)^{125}S at 25 keV in Table 6. The DC cross sections using purely theoretical input are smaller by at least about a factor of 400 than the one with experimental input. This large discrepancy arises, since there is no transition possible to the relevant final $3/2^-$– $1/2^+$ and

Table 6: Comparison of the DC cross section for ^{124}Sn(n,γ)^{125}Sn in μbarn at 25 keV with the input from the different structure models (RMFT, HFB, QRPA) and the input determined from experimental data (EXP)

J^π	RMFT	HFB	QRPA	EXP
$\frac{11}{2}^-$	0.000	0.000	0.000	0.000
$\frac{3}{2}^+$	–	–	–	43.105
$\frac{1}{2}^+$	–	–	–	69.515
$\frac{7}{2}^-$	0.015	0.036	0.038	0.023
$\frac{3}{2}^-$	–	–	–	7.697
$\frac{3}{2}^-$	–	–	–	19.687
$\frac{3}{2}^-$	–	–	–	5.148
$\frac{3}{2}^-$	–	–	–	6.987
$\sum \sigma_{DC}$:	0.015	0.036	0.038	152.162

$3/2^+$–states, which are unbound in ^{125}Sn (Fig. 2).

4 Summary

We find discrepancies by about a factor of two for the DC cross sections with input parameters from the nuclear structure models in the case of ^{36}S(n,γ)^{37}S. For astrophysical applications in nuclear–network calculations such discrepancies can be acceptable. However, for ^{124}Sn(n,γ)^{125}Sn there exists a large underestimation of the DC cross section using nuclear–structure input by at least two orders of magnitude. This is due to the higher exciation energies of the low–spin states in ^{125}Sn, compared to the high–spin states. Clearly, investigations of nuclear–structure models in the manner shown above are necessary to test the reliability of such models for the application to calculations of cross sections of astrophysically relevant nuclear reactions involving nuclei far–off stability.

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