Astrophysical S-factor calculation for selected reactions

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Abstract

Review on relevant elements of nuclear astrophysics.

Definition, motivation and applications of the astrophysical S-factor.

Survey on models that predict S-factors. They are mainly classified as empirical, potential, macroscopic and matrix models

Use of theoretical models to calculate the S-factors of selected reactions.

Comment on the applicability of the models for each reaction. Comparison between experimental data and theoretical predictions of the S-factors.

Acknowledgments

Mom for everything.

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Chapter 1

Nuclear astrophysics fundamentals

In order to apply nuclear astrophysics to the study of star element production, there are essentials to be considered. In this chapter, a general review of the main points relevant for nuclear physics are presented that emphasizes selected topics that are relevant in the field of nuclear astrophysics.

1.1 General aspects about the nucleus

Introduce a brief description of the nuclei. The structure of the nuclei The nuclear models
The nucleus is a bound state of a system of protons and neutrons. These substructures are bound states of a set of fundamental particles, which are called quarks.

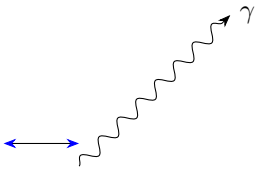
A general treatment given in [1] and basic concepts in [2].

A more particular on nuclear astrophysics [3].

Rest energy.

$$E_0 = Zm_pc^2 + (A - Z)m_nc^2 - B(A, Z), \tag{1.1}$$

where Z, A are the atomic and mass number respectively.



In addition,
Elementary nuclear structure - Atomic nuclei are bond states of nucleons They are particles Characteristics - They obey the Pauli-exclusion principle like electrons - They have magnetic moment. - They are bonded in the nuclei by the strong force which compensates the repulsive electromagnetic force - Each nucleon is conformed by elementary particles. Classification - proton: positive charge - neutron: no charge
- Mass number. Atomic number.
Leptons Characteristics - They do not interact via strong force - Considerably lighter in mass than nucleons Classification - Electron - Neutrino - Antiparticles are also considered

1.2 Elements of quantum mechanics for nuclear physics

Quantum mechanics governs the physics at the nuclear scale. In particular, some elements of quantum mechanics theory that are essential for the description of nuclear reactions. For instance, quantum mechanical treatment of scattering theory is critical for determining the behavior of the rates of the reaction. In addition, tunneling phenomena, which can only be explained from the non-classical behavior of nuclear physics, permits the existence of nuclear fusion. Finally, transition phenomena will be considered in this section from the point of view of electromagnetic transitions.
Quantum mechanics text [4].

1.2.1 Scattering theory

Explain scattering theory relevant for the understanding of processes.

The sequence of the calculations on scattering is the following - Consider free path approximation -> Bessel Function solution - Expand free wave in terms of Bessel and Harmonic oscillator solutions - Obtain the coefficients of the expansion - Evaluate asymptotic behaviour at $r \to \infty$
When considering a potential, it appears that the oscillatory asymptotic wave function is shifted $e^{2i\delta_l}$. This factor depends on the angular momentum l. This directly relates with differential cross sections.

A reference text on collision theory [5].

$$\sigma = \frac{\text{scattered per time}}{(\text{incident per time per area})(\text{total nuclei})}. \tag{1.2}$$

Cross sections are probabilities The probabilities are ruled by the laws of scattering theory, which can be understood as a subpart of quantum mechanics.
There is of interest the differential cross section. Particularly, there is a connection with quantum mechanics scattering amplitudes with the formula

$$\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2 \tag{1.3}$$

Cross section -> Reciprocal factors -> Scattering potentials -> Coloumb Barrier (With WKB approximation) -> Breit - Weigner formula (This is for resonant behavior)-> S factors, ...

There are several contributions to the total rate. There are four in principal Broad resonances, thin resonances, continuum, nonresonant. For particles of matter, the statistics at the star fusing scale is Maxwell - Boltzmann and for photons the Bose - Einstein statistics.

Scattering theory develops from the method of partial waves. It roughly consists on solving for the Schödinger equation in free space and, with the potential given, expand in terms of an orthonormal basis of functions, like spherical Bessel and Neumann functions and spherical harmonics. Then, conditions are adjusted via boundary condition satisfying.

$$\psi = \sum_l \sum_m c_{lm} Y_m^l j_l(kr) \tag{1.4}$$

Wavefunction ansatz

$$\psi = \frac{u}{r} Y \otimes \chi. \tag{1.5}$$

Free space solution with $j_l(kr)$ the spherical Bessel function of l parameter. There are also the $n_l(kr)$ Neumann function and the Hankel functions $h^{(1)}(kr)$ and $h^{(2)}(kr)$ functions.

A result that relates cross sections and the probability current density is the theorem.

$$\sigma = \frac{4\pi}{k}\mathrm{Im}(f(\theta = 0))) \tag{1.6}$$

Born approximation that is used for estimating the scattering amplitude.

$$f(\theta) = -\frac{2m}{\hbar^2}\int_0^\infty \mathcal{F}\{V(r)\}dk. \tag{1.7}$$

1.2.2 Tunneling phenomena

Quantum tunneling phenomena is critical in understanding the phenomena of alpha particles decaying in the nuclei barriers.
WKB approximation for the classical forbidden regions.

$$T = e^{2i\delta_l}. \tag{1.8}$$

Ansatz:

$$\Psi(r) = \Psi_0 \exp\left(\Phi(r)\right). \tag{1.9}$$

The Schrödinger equation transforms as

$$\left(\Phi'' + \Phi'^2\right)\Phi = \left(\frac{2m}{\hbar^2}(U(r) - E)\right)\Phi. \tag{1.10}$$

Then, if it is considered that $\Phi'' \ll \Phi'^2$, then Φ can be directly integrated and is expressed as:

$$\Phi(E) \approx -\frac{1}{\hbar}\int_{r_1}^{r_2} \sqrt{2m(U(r) - E)}dr, \tag{1.11}$$

where r_1 and r_2 correspond to the lower and higher classical turning points respectively. In this opportunity, the negative choice for the square root was taken in order to account for the fact that the probability of transmission decreases within the non-classical region.
More information in [6].

1.2.3 Perturbation theory

Generalities of perturbation theory. Cross sections. Fermi Golden rules.

$$\sigma \propto |\langle k|\delta H|m\rangle|^2 \tag{1.12}$$

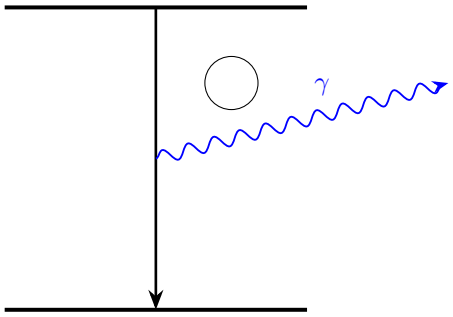
Splitting

$m_l = -1$

$l = 1$ $\qquad$ $m_l = 0$

$m_l = 1$

The changes of state that nuclei exhibit obey certain rules. In particular, this selection rules consider angular momentum conservation.



Selection rules. Electromagnetic interaction and resonances [7].

1.2.4 Angular momentum

Angular momentum is an relevant conserved quantity in physics, in particular in nuclear reactions.

1.3 Nuclear structure

Nuclear structure is presented in this section.

1.3.1 Nuclear models

Stability depends closely on the biding energy. In particular, since the rest energy of the nucleus decreases with $B(A, Z)$, the more is the binding energy, the more stable is nucleus.

Liquid drop model

A first approach when modeling the binding energy is a phenomenological model which is inspired in the physical description of a liquid drop. In particular, the predictions of the binding energies are determined by the fitting of the empirical formula:

$$B(Z, A) = a_v A - a_s A^{2/3} - a_3 \frac{Z(Z+1)}{A^{1/3}} + a_4 (Z - A)^2 + a_5 \delta. \tag{1.13}$$

However, this model does not fit accurately the binding energy of a selected nuclei which are more stable than expected from the model. In particular, it is said that the pair of number of protons and nucleons (Z, A) of these nuclei are magic numbers.
- The more stable the nuclei, the greater the binding energy. Binding energy is the energy difference of rest energy of the nucleus constituents and the actual rest mass of the overall nucleus.

$$\delta = \begin{cases} 1, & Z \text{ and } A \text{ even} \\ -1, & Z \text{ and } A \text{ odd} \\ 0, & \text{otherwise} \end{cases} \tag{1.14}$$

Nuclear shell model

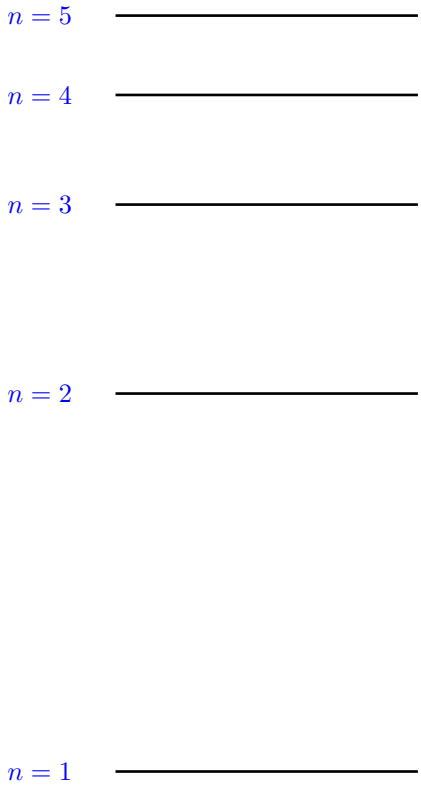
An alternative approach to the Liquid drop model is a model based on quantum mechanics. This model is closely related with the quantum mechanical modeling of the hydrogen atom. In particular, a great part of the nuclear shell model consists of solving Schrodinger equation which is expressed as:

$$-\frac{\hbar^2}{2m}\partial_{tt}\psi + V\psi = E\psi. \tag{1.15}$$

In this case, the potential V represents the effective potential of the core of the nucleus and is valid at certain radii. For example, the harmonic potential $V = m\omega^2 r^2$ models effectively the system of nucleons at most regimes.

Spin orbit coupling rules the energy levels of the nucleons.

- Nuclear shell model is based on quantum mechanics.
-Nuclear shell model can predict the existence of the magic numbers.

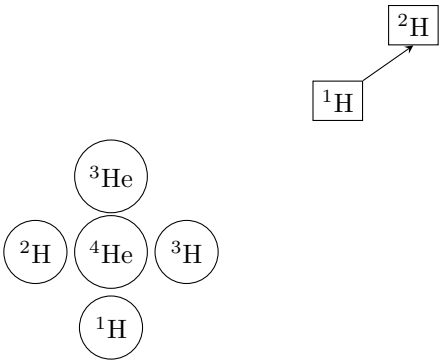


1.3.2 Nuclear levels and transitions

Nuclear levels work in a similar way than atomic levels. Additionally, the are possibilities of transitions between levels.

1.4 Nuclear reactions

Nuclear reactions are reactions between nuclei. [8].



1.4.1 Classification of reactions

The relevant reactions for the document are:

$$0 + 1 \rightarrow 2 + 3 \tag{1.16}$$

$$\gamma + 3 \rightarrow 0 + 1 \tag{1.17}$$

Expand on how the fusion reactions occurs, their conditions and types as well as the differentiation factors with respect to fission processes.

Capture reactions

Also, radiative capture processes are considered at astrophysical energies. Various models could be used for determining potentials. There are clusters and potential models.

$$X + c \rightarrow \gamma + X'. \tag{1.18}$$

When c is a proton, the reaction is called radiative proton capture. [9]

Exchange reactions

$$X + x_1 \rightarrow x_2 + X' \tag{1.19}$$

A development on the (p, n) reaction kind is given by [10] and for the (n, p) in [11].

Fusion reactions

$$X + X \rightarrow a + X'. \tag{1.20}$$

1.4.2 Cross sections

Cross section of a process. Partial and total cross sections depending on the reaction type. Cross sections have relations with the S-matrix.

1.4.3 Reaction rates

The ratio that determines the quantity of a nucleus.

$$r = A \int_0^\infty E\sigma(E) \exp\left(-\frac{E}{kT}\right) dE. \tag{1.21}$$

$$P(v)dv \propto v^2 \exp\left(\frac{mv^2}{2kT}\right) dv. \tag{1.22}$$

On specifying the rates, it is needed to be considered.
Reaction rates are considered from calculation of transmitted, incident and interacting - Reaction rate depends on the density of particles, the velocity and the cross section - It is averaged by a convenient distribution. (Maxwell-Boltzman for fermions, Bose Einstein (Planck) for photons) - With the rates, abundance evolution is determined
There are broad classification of reactions.

1.5 The Astrophysical S-factor

Cross section does not count for the low-energy behavior. Then, additional factors can be obtained. For example, S-factor.

1.5.1 Motivation and definition

There are S factors associated with the energy and they are the path to determine the nature of the potential, which is not necessarily a Yukawa potential.

$$S(E) = E \exp(2\pi\eta)\sigma(E). \tag{1.23}$$

It is directly proportional to the microscopic cross section of the process $\sigma(E)$ and it represents the rate of a certain nuclear reaction. In particular, the astrophysical S-factor scales the cross section with a factor proportional to the Coloumb repulsion.
The ν factor is defined as

$$\eta = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 \hbar v} \tag{1.24}$$

where v corresponds to the relative speed between the reactants.
There is a strong relation of the astrophysical S factor with the center of mass energy.
Usually this relation depends on the square of the energy of the center of mass E_{cm}.

There are topics that are relevant in the frontiers of nuclear astrophysics [12].

1.5.2 General applications

Cross section extrapolation to low energies
Reaction rates and element abundance estimations.

Chapter 2

Reactions of astrophysical interest

Nuclear reactions are part of the core of nuclear astrophysics. They are accountable for the production mechanism of elements in several astrophysical environments where thermonuclear reactions can occur. In particular, there are specially relevant reactions for the explanation of the abundance of elements. For example, some of these reactions are part of critical fusion chains of stars, have challenging extrapolation techniques to low energies, or exhibit exotic underling physical phenomena.

In this section, a relevant selection of reactions types of will be reviewed. Several reaction kinds and models are given in [13].

2.1 Big Bang nucleosynthesis

Primordial reactions that where expected to happen just after the Big Bang occurred. For example:

$$^{2}\mathrm{H} + \mathrm{p} \rightarrow \gamma + {}^{3}\mathrm{H}. \tag{2.1}$$

BBN description [14] Review [15].
Elements very high temperatures [16]
CNO elements BBN [17].
Lithium problem [18].

2.2 Stellar fusion

The classical treatment of fusion in stars is given by the classical [19].
Summary [20].
Hertzsprung-Russel diagram [21].
Introduce the needed conditions for the creation of stars in the primordial nebula. Describe how the hydrogen is burnt in the star's core and the associated products.

$$p + p \rightarrow d + e^{+} + \nu_e. \tag{2.2}$$

Consider the mechanisms for exchanging heat via radiation and convection.
Explain the required conditions that permits nuclear fusion in the star's nucleus.

2.2.1 Light heavy nuclei reactions

pp chain

pp chain review [22].

Triple alpha process

Triple - alpha process review [23].

Alpha ladder

Alpha reactions Ne cycle [24].
This reaction is governed by the weak force, due to conversion of a proton into a neutron, and by the strong and electromagnetic force.
When it comes to deuterium fusion, this channel is the most abundant.

$$d + d \rightarrow n + {}^{3}\mathrm{He}. \tag{2.3}$$

The reaction rates of nuclear fusion processes depend on the interaction cross section and the abundance of the reactant nuclei.

$$d + d \rightarrow p + t. \tag{2.4}$$

The interactions of the previous processes are the electromagnetic and strong force.

$${}^{3}\mathrm{He} + p \rightarrow {}^{4}\mathrm{Li} + \gamma \rightarrow {}^{4}\mathrm{He} + e^{+} + \nu_e + \gamma. \tag{2.5}$$

This process is unlikely because of the instability of ^{4}Li, which decay to ^{3}He.

$${}^{3}\mathrm{He} + {}^{3}\mathrm{He} \rightarrow {}^{4}\mathrm{He} + 2p. \tag{2.6}$$

This process in known as the pp1 chain.
Exemplify how the reaction mechanisms permits the stability of a star as well as produces He.

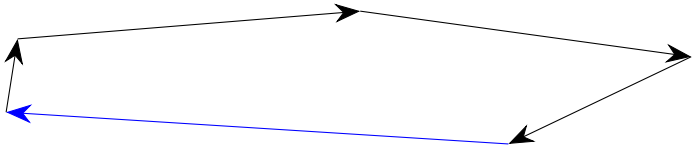
Screening effect present in light weight nuclear reactions [25] and a review of screening effect [26].

2.2.2 CNO cycle

The carbon burning produces the neutrons that are going to be used in heavy nuclei production. The neon burning stats by fusion Neon nuclei with 4He nuclei to produce heavier elements. The oxygen burning starts are very high temperatures and pressures than the neon and carbon burning due to the high stability of oxygen nuclei. In fact, oxygen nucleus is double magic.

CNO cycle reactions [27].
When the star has capacity for producing elements like carbon, oxygen and nitrogen, CNO cycle process can be produced. In particular, reactions take the form

$${}^{12}_{6}\mathrm{C} \rightarrow {}^{13}_{7}\mathrm{N} \rightarrow {}^{13}_{6}\mathrm{C} \rightarrow {}^{14}_{7}\mathrm{N} \rightarrow {}^{15}_{8}\mathrm{O} \rightarrow {}^{15}_{7}\mathrm{N} \rightarrow {}^{12}_{6}\mathrm{C}. \tag{2.7}$$



There are other CNO cycles that involve oxygen and fluorine reactions. For instance, the second CNO cycle consists of the following reactions

$${}^{15}_{7}\mathrm{N} \rightarrow {}^{16}_{8}\mathrm{O} \rightarrow {}^{17}_{9}\mathrm{F} \rightarrow {}^{17}_{8}\mathrm{O} \rightarrow {}^{14}_{7}\mathrm{N} \rightarrow {}^{15}_{8}\mathrm{O} \rightarrow {}^{15}_{7}\mathrm{N}. \tag{2.8}$$

There is even a CNO III cycle, which is far more uncommon. brig This branch is less dominant than the first branch.

2.2.3 Medium heavy fusion reactions

These reactions concern nuclei with $A < 28$. Examples of this kind of reaction include the $^{12}\mathrm{C} + {}^{12}\mathrm{C}$, $^{12}\mathrm{C} + {}^{16}\mathrm{O}$ and the $^{16}\mathrm{O} + {}^{16}\mathrm{O}$ fusion reactions. Most of these reactions result in different channels.

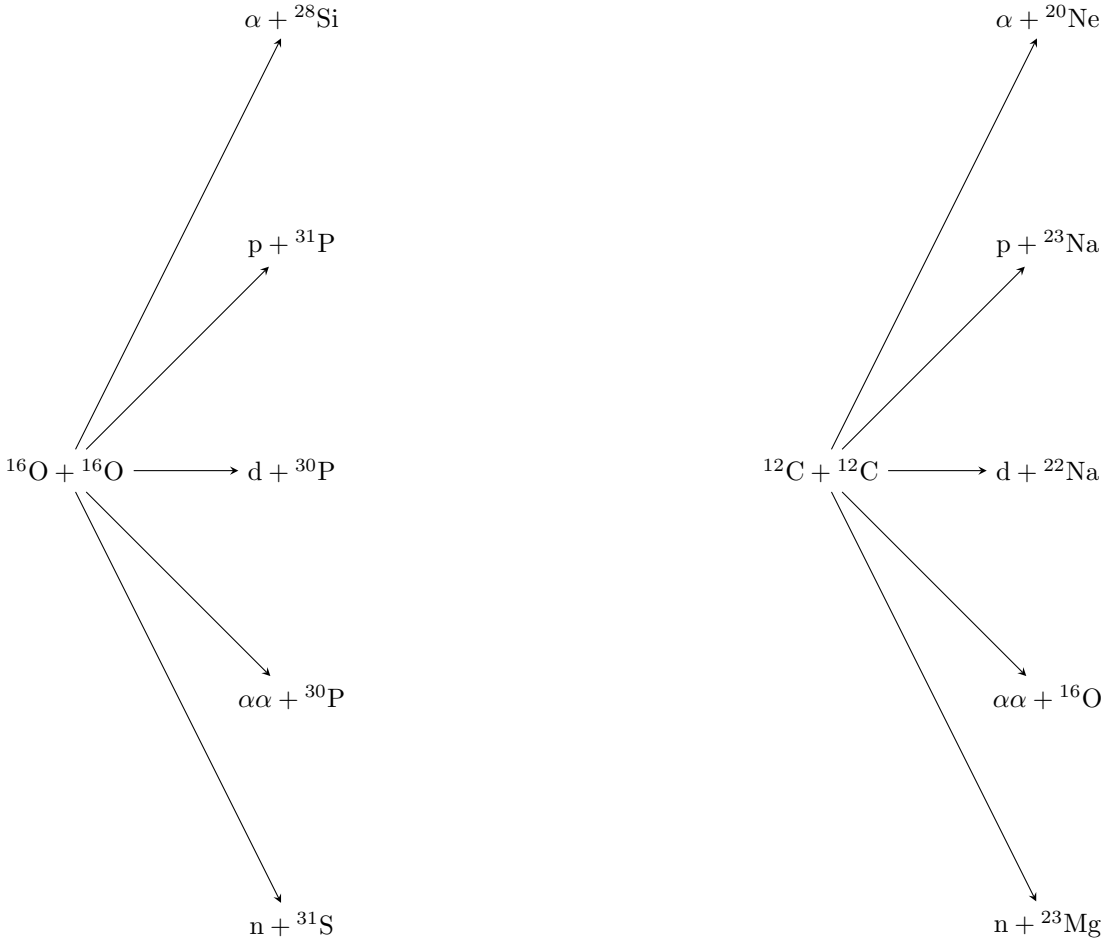
With respect to the carbon fusion reaction, the principal channel is given by:

$$^{12}\mathrm{C} + {}^{12}\mathrm{C} \rightarrow {}^{4}\mathrm{He} + {}^{20}\mathrm{Ne}. \tag{2.9}$$

On the other hand, the main channel of the oxygen fusion reaction occurs in the following manner:

$$^{16}\mathrm{O} + {}^{16}\mathrm{O} \rightarrow {}^{4}\mathrm{He} + {}^{28}\mathrm{Si}. \tag{2.10}$$

Additionally, there are inelastic channels associated with $^{16}\mathrm{O}$ which could increase the probability of occurrence for the overall reactions.



There are more cycles of capture reaction. An example regarding the MgAl cycle is given in [28].
There is a silicon burning process with the following description

$$^{28}_{14}\mathrm{Si} + {}^{4}_{2}\mathrm{He} \rightarrow {}^{32}_{16}\mathrm{S}. \tag{2.11}$$

Silicon burning is another process.

$$^{28}\mathrm{Si} + {}^{28}\mathrm{Si} \rightarrow {}^{4}\mathrm{He} + {}^{56}\mathrm{Fe}. \tag{2.12}$$

Fusion up to oxygen [29].
Nucleosynthesis in massive stars [30]
Neon burning [31].
Silicon burning [32].
12C + 12C Wave packet dynamics[33] nonresonant Bayersian [34] Modified sfactor [35] Trojan horse [36] [37] full-microscopical [38] multichannel folding [39] screening effects [40]
correlation between carbon fusion reactions [41] constraint 12C + 12C based on 12C + 13C reaction [42]
16O + 16O cross sections [43] [44]
oxygen isotopes fusion [45] coupled channels [46]
12C + 16O semi-microscopic cluster [47] low-energy resonances [48] 12C + 16O based on yields of 12C + 16O and 12C + 18O [49]
selected oxygen-oxygen and oxygen-carbon reactions [50] [51] 12C + 12C and 16O + 16O [52]
12C and 24 Mg resonances [53] Fusion hidrance 12C + 24Mg [54]

2.3 Heavy nuclei reactions

Explain the different chains going on during the carbon-oxygen combustion to heavier elements like iron or silicon.
Additional fusion reactions with nuclei with $A > 28$ are present at the last stages of the life of a star. There are two main environments: The stellar fusion and explosive events fusion.
heavy-ion reactions [55]

2.3.1 Supernovae and other explosive environments

This reaction is essential since the ^{56}Fe nucleus has the maximum binding energy. Then, fusion reactions of heavier nuclei tend to be less spontaneous.Then, this chain of reactions continues until the process in there 56-Ni is reached.

2.3.2 Alpha reactions

$$^{52}_{26}\mathrm{Fe} + {}^{4}_{2}\mathrm{He} \rightarrow {}^{56}_{28}\mathrm{Ni}. \tag{2.13}$$

Alpha and cluster decay [56].
Alpha induced reactions [57].

2.3.3 The s and r processes

There exists the s and the r processes. Each permits to form heavier nuclear elements products. Now, there are aspects of the particularities of the production of the nuclei that are currently unknown

On the other hand, protons are captured at the ending of the life of a gigantic star. This process, which occurs at high densities and temperatures, is referred as proton capture. In particular, under astrophysical scenarios like supernovas, the rapid proton capture, in addition to the neutron capture, produces a considerable amount of the heavy nuclei. This process is referred as rapid proton capture, or rp process.

Further processes are not viable because they are not exothermic and potential heavier nuclei than 56-Ni are photodisintegrated. At this scale of energy, nuclear reactions start to behave similarly than chemical equilibrium reactions.

The conditions are associated with the mass. Particularly, depending on the mass regime, star evolution can differentiate. For instance, there are brown dwarfs, sun like stars.

There is an evolution process that is ruled by different instances. Each instance can be regarded as a region in the Hertzsprung-Russell diagram. This diagram consists of a two dimensional scatter plot of the intensity with respect to the spectral type of a star. Particularly, there are regions associated to the different instances of the life of a star: Main sequence (Hydrogen burning stars), red stars, neutron stars, supernova of kinds Ia Ib and other instances.

Electron degeneracy prevents the white dwarf to collapse and the neutron degeneracy pressure prevents the neutron star to collapse. These limits account for relativistic Fermi gas and neutron degeneracy with a model from general relativity.

Indicate that there exists different channels of production depending on the existence of neutron capture or fission products. Additionally, explain the needed conditions in order to those processes to occur.

If mass increases further, there is no place to any degeneracy compensation so the star would collapse to a black hole.
s-process known and unknown [58].
s-process nucleosynthesis [59].
r-process form O-Ne-Mg cores [60].
r-process and beta decay [61].
alpha-process and r-process [62].
r-process without excess neutrons [63].
Neutrino capture and r-process [64].
r-process production beyond ^{209}Bi [65].
Electron capture [66].

2.3.4 The p and rp processes

The p processes are proton capture process.

The rp processes are like the p processes going on in a faster rate.
Abundance p-process [67].
Proton drip-line middle-heavy nuclei [68].
Alpha - gamma heavy p-nuclei [69]
Proton and alpha capture p process [70] [71].
p-process nuclei [72]
End point rp processes [73].
Proton drip-line rp processes [74].

2.4 Active research topics

Enumerate the broad ranges of phenomena that are left to be explained.

Introduce current approaches of some of the unsolved questions on nuclear astrophysics, particularly on the last instances of fusion in the star's lifetime.

There are various types of supernovae. However, there are mechanisms that are not considered and yet not well explained.

Current experiments in detection of heavy nuclei are essential to determine the distribution of elements, specially in events like the fusion of neutron stars.

Heavy and superheavy nuclei production [75].
Review on active research topics and current challenges in nuclear astrophysics in general [76] and on low-energy nuclear physics [77] are given.

Chapter 3

Astrophysical S-factor models

There are several methods for estimating the astrophysical S-factor. Each method is more convenient depending on the nature of the reaction. For example, method accuracy can vary depending on the reaction type or the existence of resonant phenomena. Additionally, the methods are based on a specific approach when modeling the S-factors. In this section, the principal methods of estimating the astrophysical S-factors will be reviewed.

3.1 Microscopic models

Microscopic models are based on first principles and usually require assumptions about the nucleus and its structure.

$$H = \sum_k T_k + \sum_k V_k(r) + \sum_{k \neq j} V_{kj}(r). \tag{3.1}$$

Modern theories [78]

3.1.1 *Ab initio* models

These models start from first principles without prior empirical or phenomenological assumptions. On the other hand, clusters consider the system of interactant nuclei as a whole. In particular, there are models based on *ab initio* assumptions about a particular set of nuclei.

Ab initio [79] [80] [81] [82] tensor force [83]
The *ab initio* no core shell model is presented in [84].

3.1.2 Many body models

The nucleus can be modeled as a many body system. Naturally, the nucleons are the components of this bounded system. In addition, the interactions between the components of the nucleus are nuclear interactions of a certain shape and form.

These models take into account the different bodies that make up the nuclei.

Therefore, cross section determination is reduced to the analysis of a many body quantum mechanics problem with all the nuclear compounds.

Multi-body calculations. Non-local calculations.

Also, nuclei deformation can be considered in models. For example, there are models with no-core shell.

Three body [85]
No core shell model [86]
Hauser-Feshbach [87]
Hartree-Fock [88]

3.1.3 Cluster models

Despite the fact that many body microscopical models are general enough to explain many kinds of nuclear phenomena, calculations may be complex to perform as the number of nucleons growth. Therefore, in order to tackle the complexity issue, physically consistent models with less constituents are needed.

One proposal for reducing the number of entities is to model the nucleus as a bounded system of clusters. A cluster is a selected subsystem usually composed by more than one nucleon. Then, the nucleus at large is represented by the resulting cover of all of its clusters.

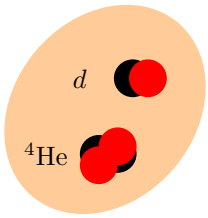


Figure 3.1: Artistic representation of a clustered ^{6}Li nucleus. The nucleus covers a two cluster system with an α particle and a deuterium as its constituencies.

An example of clustering is given with the ^{6}Li nucleus depicted in Figure 3.1. With this picture, it is observed how the number of interacting bodies has decreased from 6 nucleons to 2 clusters: the ^{4}He and deuterium nucleus.

Additionally, it is said that the α particle and the deuterium nucleus are the core and the valence clusters respectively. This classification is analogous to the core and valence electrons used in atomic physics. In particular, the core corresponds to the α particle cluster since it has more nucleons than the valence cluster which is the d nucleus.

On the other hand, in order to give this kind of models physical significance, selected interactions between clusters are introduced. The NN and NNN forces are standard examples of such needed interactions. In addition, since the constituents usually have many nucleons, extended object parameters like mass and charge density distributions may be encountered.

The mass and nuclear density of the nuclei can be modeled as a Woods-Saxon distribution as follows:

$$\rho(r) = \frac{\rho_0}{1 + \exp\left(\frac{r-R}{a}\right)}. \tag{3.2}$$

With folding.

$$\int\int \rho(r_1)\rho(r_2)dr_1dr_2. \tag{3.3}$$

A more detailed survey on cluster models [89].
Microscopical cluster light nuclei [90].
Alpha-cluster alpha-closed shell [91].
Shell model [92] [93]
Multicluster [94] [95]
Break up effects [96]
Linear chain [97]

3.2 Matrix models

The matrix models permit the modeling of resonances with an appropriate fitting of free parameters. In particular, the main formalism in this approach is the R-matrix model [98] [99].

On the other hand, there are matrix models with no free parameters. For example, the K-matrix model predicts the cross sections without including the channel radius, which is an arbitrary parameter required in the R-matrix calculations [100].

Finally, there is more than a single parametrization for matrix models [101]. Usually the alternative formulations surge from the need to express the parameters of the model in order to facilitate the imposition of boundary conditions.

3.2.1 Calculable R-matrix

The model includes free parameter a which is called the radius channel.

$$R_{cc'} = \sum_k \frac{\gamma_{ck}\gamma_{c'k}}{E - E_k}. \tag{3.4}$$

The sum is over levels and the elements are parameterized as channels.

Resonances arrives from poles. A description on the physical consideration of poles in the scattering (S-matrix) is given in [102].

Applications of the R-matrix formalism to specific reactions:
In primordial nucleosynthesis [103] big-bang 3He and several reactions [104].

Bayesian fitting methods [105].
Litium detueron capture [106].

10B proton non-radiative [107] and similarly [108]. 10B radiative and resonances in 11C inverse kinematics [109].
Alpha capture reactions of carbon [110]. Hybrid potential/R-matrix [111].
13C alpha capture and 16O determination [112].
Proton capture carbon [113] for C12 and [114] for C13 and [115] for the same reaction .

15N capture in [116] and 14N in [117]. also on 14N proton capture [118].

3.2.2 Phenomenological R-matrix

The penetration factor parameter $P(E)$ which is expressed as:

$$P = \frac{\Gamma}{F_l^2 + G_l^2}, \tag{3.5}$$

where the functions $F_l = F_l(ka)$ and $G_l = G_l(ka)$ are the Coulomb functions evaluated at a particular $\rho = ka$. In addition, another parameter Q is given:

$$Q = \frac{\Gamma}{F_l G_l' + G_l F_l'}. \tag{3.6}$$

On the other hand, the phase shift is given by:

$$\delta = \delta_{\text{HS}} + \delta_R. \tag{3.7}$$

An empirical formula obtained from the R-matrix formalism is given by:

$$S(E) = S_r \frac{\Gamma^2/4}{(E - E_r + \Delta)^2 + (\Gamma/2)^2}. \tag{3.8}$$

3.2.3 K-matrix

There is also the K-matrix model as an alternative of the R-matrix model [100]. The advantage of this model with respect to the R-matrix is that the K-matrix does not include the channel radius as a free parameter. Alternative formulation of R-matrix [101].

3.3 Potential models

Nuclei are considered as objects subject to effective interactions. These interactions are also modeled by effective potentials which account qualitatively for the nature of the underlying physics behind the nuclear reactions. In particular, different kind of potentials offer a particular shape of the interaction which make them suitable for the modeling of concrete reactions.

3.3.1 Effective potentials

The effective interaction between nuclei is referred as a composite effect of the electromagnetic and nuclear interactions.

The first interaction is considered due to the electromagnetic repulsion between the nuclei. In a first approach, the substructure of the nuclei is ignored. Then, nuceli charged cloud is modeled as uniformly charged sphere. Therefore, the corresponding potential is given by:

$$V_{\text{EM}} = \begin{cases} \dfrac{Z_1 Z_2 e^2}{4\pi\epsilon_0 R}\left(\dfrac{3}{2} - \dfrac{r^2}{2R^2}\right), & r \leq R \\ \dfrac{Z_1 Z_2 e^2}{4\pi\epsilon_0 r}, & r > R \end{cases} \tag{3.9}$$

Secondly, in order to account for the nuclear force, an short-distance attractive potential is needed to be included. However, unlike the electromagnetic interaction, nuclear potentials might not be deduced in a closed and fundamental form such as the expression given in 3.9. Consequently, these potentials are usually phenomenological and account for specific purposes. In fact, there is a an extent list of potentials available in literature which are used for modeling the interactions of different kind of reactions.

For instance, in a first approximation, there is the step potential.

$$V_{\mathrm{SqW}} = -V_0\theta(r). \tag{3.10}$$

Yakovlev et. al model [119] consists of an estimation of the potential that is similar to the parabolic potentials with free parameters that attempt to account for the effects of the nuclear and electromagnetic interactions.

$$V_{\mathrm{YAK}} = \begin{cases} E_c\left(3 - \dfrac{r^2}{R_c^2}\right), & r \leq R_{c1} \\ \dfrac{Z_1 Z_2 e^2}{r}, & r > R_{c1} \end{cases} \tag{3.11}$$

Additionally, the model distinguish between classical allowed and forbidden regions. For the first region, where $E < E_c$, the astrophysical S-factor is estimated as:

$$S(E) = S(0)\sqrt{\frac{Ec}{E}}[\exp\left(\Psi(E)\right) + k\xi], \tag{3.12}$$

where ξ is a free parameter of the model that accounts for the deviation from free particle behaviour of the S-factor. On the other hand, $S(0)$ corresponds to the zero-energy extrapolation of the S-factor.

uses the WKB approximation for estimating the wave function. Then, the astrophysical S-factor is determined by a phenomenological equation.

$$\Psi(E) = 2\pi\eta(E) + \Phi(E), \tag{3.13}$$

where $\eta(E)$ is the Sommerfeld parameter, and $\Phi(E)$ is the wavefunction calculated by the WKB. Further details on the calculation of the last parameter are presented in section 1.2.2.

In order to the potential to be more realistic, a Woods-Saxon potential consider a smooth behavior.

$$V_{\mathrm{WS}}(r) = \frac{V_0}{1 + \exp\left(\frac{r-R}{a}\right)}, \tag{3.14}$$

where V_0 represents the potential depth, a the parametrization and R a computed radius which is defined as:

$$R = r_0(A_1^{1/3} + A_2^{1/3}). \tag{3.15}$$

On the other hand, it is relevant, specially at low energies, the inclusion of angular momentum effects in the potential. In order to account for that effect, there is the potential with angular moment.

Also, spin orbit coupling effect is noticeable for certain kind of reactions. The contribution to the potential associated with this effect is expressed as:

$$V_{\mathrm{SO}}(r) = k\langle L \cdot S\rangle \frac{1}{m_\pi r}\frac{d}{dr}V(r), \tag{3.16}$$

where the coupling $\langle L \cdot S\rangle$ is expressed as:

$$\langle L \cdot S\rangle = J(J+1) - l(l+1) - s(l+1). \tag{3.17}$$

Double exponential potentials:

$$V_{\mathrm{DE}}(r) = -V_0\left(e^{\alpha_1 r} + e^{\alpha_2 r}\right)^{-1}. \tag{3.18}$$

Cluster potential:

$$V_{\mathrm{CL}}(r) = -V_0 \exp\left(-\alpha r^2\right) + V_1 \exp\left(\beta r\right). \tag{3.19}$$

Gaussian exponential:

$$V_{\mathrm{GE}}(r) = -V_0 \exp\left(-\alpha r^2\right). \tag{3.20}$$

Yukawa potential which includes screening effect.

$$V_{\mathrm{Y}} = -\frac{c}{4\pi\epsilon_0} e^{-\mu r}. \tag{3.21}$$

3.3.2 Calculations

The potentials just introduced are useful for the calculation of cross sections and, therefore, S-factors. The connection between potentials and cross sections depends on the kind of reaction to be modeled. In the general approach, cross sections are directly computed form wave functions, which are numerically estimated from the numerical solution of the Schroödinger equation.

On the other hand, in certain specific cases when the expressions of the potentials are not mathematically sophisticated, approximations can be made. In particular, WKB approximation offers a comprehensive approach towards handy estimation of the cross sections.
In the radiative capture reactions, cross sections are computed based on electromagnetic field operators. In particular

$$\sigma_m = \sum_k \langle k|\mathcal{O}|m\rangle C_{klm}. \tag{3.22}$$

3.3.3 Folding

During the previous discussion, mass and charge distributions were not considered in detail. However, with nuceli with higher mass, the intrinsic distribution of the mass and charge gains relevance in the reaction cross section estimation. In particular, mass and charge is usually concentrated at the center of the nuceli and there is a sharp drop of the mentioned variables in the surrounding of the radius.

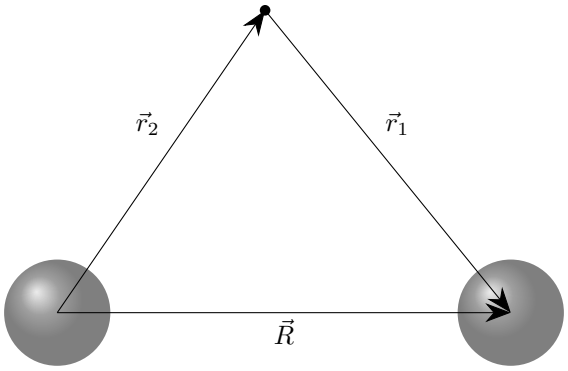
In order to account for this effect, an initial formula which accounts
Sao pablo [120]

$$V_{\mathrm{SPP}}(r) = V_{\mathrm{F}}(r) e^{-4V^2/c^2}. \tag{3.23}$$

$$V^2 = \frac{2}{\mu}\left(E - V_{\mathrm{F}}(r) - V_{\mathrm{C}}(r)\right), \tag{3.24}$$

where the reduced mass is μ, the Coulomb potential is $V_{\mathrm{C}}(r)$ and the folding potential $V_{\mathrm{F}}(r)$ is expressed as:

$$V_{\mathrm{F}}(r) = \int\int \rho_1(\vec{r}_1)\rho_2(\vec{r}_2)\delta(\vec{r} - \vec{r}_1 + \vec{r}_2) d\vec{r}_1 d\vec{r}_2. \tag{3.25}$$



3.3.4 Non-locality

And, potentials with non-locality are also found in literature. For example, there is the São Pablo potential that accounts for the effect of non-local interactions between the interactant nuclei.

Capture reaction review light nuclei[121] [122]
7Be radiative capture [123] [124]
9Be radiative capture [125]
p2H radiative capture [126]
2Hdp reaction [127]
13C radiative capture [128] [129]
11C radiative capture[130]
16O fusion [131]

Optical model [132]

$$V(r) = V_R(r) + iW_R(r). \tag{3.26}$$

Woods-Saxon [133] [134]

$$V_{\mathrm{WS}} = -V_0 f(r), \tag{3.27}$$

$$f(r) = \frac{1}{1 + \exp\left(\frac{r-R}{a}\right)}. \tag{3.28}$$

Energy dependent model [135]
$V_0(E)$
Cross section deduced potential [136] [137]

3.4 Special models

Models which do not fit in the previously presented categories.

3.4.1 Trojan Horse models

It occurs in a two step reaction process as expressed in:

$$A + B \rightarrow a + b \rightarrow a + (c + d), \tag{3.29}$$

where the first and second steps correspond to the $A + B \rightarrow a + b$ and $b \rightarrow c + d$ reactions respectively. Notice that the b nucleus does not appear as a final product of the reaction as it is consumed in the second step. The Trojan horse method [138].

3.4.2 Effective field theories

Based on effective field theories. The general principle of these theories is that nuclear interactions correspond to low-energy approximate solutions of the physics described in quantum chromodynamics.

$$\mathcal{L} = N^{\dagger} i\hbar\gamma^{\mu}\partial_{\mu}N + ... \tag{3.30}$$

Diagrams associated with the processes of low-energy nuclear force. Mediators are mesons like pions.

Effective field theory [139] [140].

3.4.3 Hybrid models

These models include aspect of potential, microscopical and even R-matrix models. For example, there are models with clustering and effective potentials.

3.5 Empirical formulas

And some empirical formulas can be given.

3.5.1 Interpolations

Non-resonant reactions S-factors can be calculated with polynomial interpolations and fits.
In particular, there is a polynomial expansion that is reported in literature to be useful.

$$S(E) = \exp\left(g_0 + g_1 E + g_2 E^2 + g_3 E^3 + ...\right). \tag{3.31}$$

Also, more generic expansions are modeled by fitting a Laurent series expansion.

$$S(E) = \frac{a_{-1}}{E} + a_0 + a_1 E + a_2 E^2 + ... \ . \tag{3.32}$$

For most of the reactions, $a_{-1} = 0$, since $S(E)$ should be smooth at very low energies. Therefore, the S-factor is described as a Taylor series expansion.

$$S(E) = a_0 + a_1 E + a_2 E^2 + ... \ . \tag{3.33}$$

3.5.2 Fusion reactions formulas

Fusion reactions, which is a more sophisticated model [141].

$$S(E) = \sum_{k=0}^{N} a_k E^k + \left(1 + \exp\left(1 + \frac{E - E_c}{D}\right)\right)^{-1} \sum_{l=0}^{M} b_l E^l. \tag{3.34}$$

3.5.3 Resonances and composite formulas

For resonant reactions, the Breit-Wigner formula

$$S(E) = S_r \frac{\Gamma_r^2/4}{(E - E_r)^2 + (\Gamma_r/2)^2}. \tag{3.35}$$

This formulation permits empirical formulas to add resonant terms to the non-resonant estimation. Usually the resonant terms are added to background which is fitted to a non-resonant formula. For example, consider the expression:

$$S(E) = \sum_{k=0}^{N} a_k E^k + \sum_{l=1}^{M} \frac{\Gamma_l^2/4}{(E - E_l)^2 + \Gamma_l^2/4}, \tag{3.36}$$

Analogously, if the non-resonant term has a polynomial form, the S-factor hybrid resonant and non-resonant expansion is expressed as:

$$S(E) = \exp\left(\sum_{k=0}^{N} a_k E^k\right) + \sum_{l=1}^{M} \frac{\Gamma_l^2/4}{(E - E_l)^2 + \Gamma_l^2/4}, \tag{3.37}$$

where N is the maximum order of the polynomial to be fitted, which accounts for the non-resonant behavior of the reaction, and M represents the number resonances present in the reaction.
Applications in direct capture [142]. Exchange reactions (p, n) kind [143].
Charged particle collisions non-resonant [144] and resonant [145].

Chapter 4

S-factor calculations for selected reactions

In this chapter, the S-factor calculation for a selected list of reactions will be presented. The list of reactions distinguish between resonant and non-resonant reactions. Additionally, this list includes reactions from Big Bang nucleosynthesis, pp-chain, CNO cycle and middle heavy nuclei fusion astrophysical environments.

In order to account for the best predictions for the astrophysical S-factors of the referred reactions, a motivation on the selection of a particular model will be mentioned, as well as the calculation consideration used to perform the calculations will be detailed for each reaction.

Further details about capture reactions with single-particle states is given by [146].

Additional, about pp-chain is given by [147].
Computer libraries that were used:
Python [148], Pandas [149], NumPy [150], SciPy [151], Matplotlib [152].

4.1 Non-resonant reactions

The starting point in the process of analysis of reaction is the study of its non-resonant part.

Light heavy selected reactions are $^{2}\mathrm{H}(\mathrm{p},\gamma)^{3}\mathrm{He}$ and $^{2}\mathrm{H}(\mathrm{d},\mathrm{p})^{3}\mathrm{H}$. On the other hand, $^{12}\mathrm{C}+{}^{12}\mathrm{C}$ and $^{16}\mathrm{O}+{}^{16}\mathrm{O}$ are the fusion reactions to be considered.

Empirical formulas are initially considered for the light heavy S-factor description. In particular, the non-resonant part of the equations 3.37 and 3.36 are fitted to experimental data.

In addition, a correction factor that accounts for the electron screening effect observed at low-energies in the $^{2}\mathrm{H}(\mathrm{d},\mathrm{p})^{3}\mathrm{H}$ reaction is included.

On the other hand, fusion reactions are described by the Yakovlev et. al empirical formula [141] and potential model [119].
Microscopical and matrix model approaches are used to be describe all the selected reactions.

4.1.1 Calculation considerations

Empirical formulas were determined by fitting parameters to best describe experimental data. In particular, the parameters chosen minimized the chi-squared χ^2 function as it is described in appendix C. In some cases, it was necessary to constraint the interval of validity of the parameters in order to avoid unphysical behaviour of the fittings. Further details about this constraints can be found in section C.2.

For the case of Yakovlev et. al potential model, an analytical calculation was performed. In this calculation, the parameters given in [119] were used for the selected fusion reactions.

In the Yakovlev model, there is a fitting of the parameters in the following way. The free parameters are δ, E_c and ξ. In particular, E_c can be determined by the following expression:

$$E_c = \frac{\alpha}{R}, \tag{4.1}$$

where $\alpha = \sqrt{Z_1 Z_2 e^2}$ and R is a parameter that is determined as:

$$R = R_0 + \Delta R_1 |2Z_1 - A_1| + \Delta R_2 |2Z_2 - A_2|. \tag{4.2}$$

In particular, the parameter R_0 depends on the reactant nuclei while the parameters ΔR_1 and ΔR_2 can assume two values per pair of reactant nuclei. For instance, the values are given in the following way:

$$\Delta R_1 = \begin{cases} \Delta R_{10}, & 2Z_1 > A_1 \\ \Delta R_{11}, & 2Z_1 < A_1 \end{cases} \tag{4.3}$$

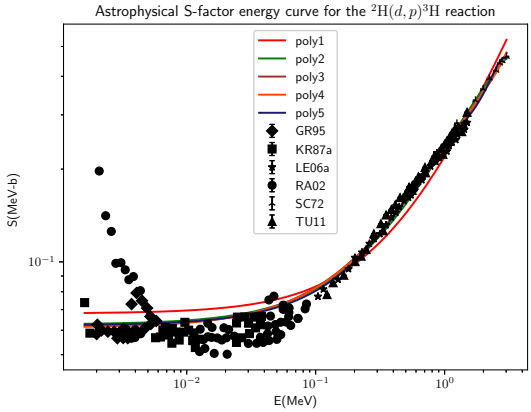
Analogously, ΔR_2 is determined as:

$$\Delta R_2 = \begin{cases} \Delta R_{20}, & 2Z_2 > A_2 \\ \Delta R_{21}, & 2Z_2 < A_2 \end{cases} \tag{4.4}$$

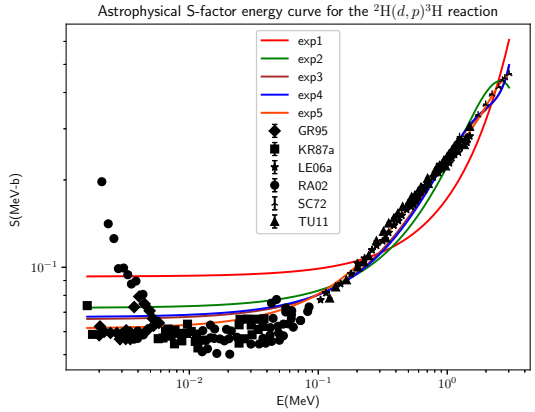
The numerical values that were provided in [119] for each of the reactions to be studied are contained in section A.4.

Although Yakovlev et. al model is used for middle-heavy fusion reactions, is not expected to work for radiative capture reactions since it predicts a decrement of the S-factor for all energies. In contrast, the S-factor increases in radiative capture reactions.

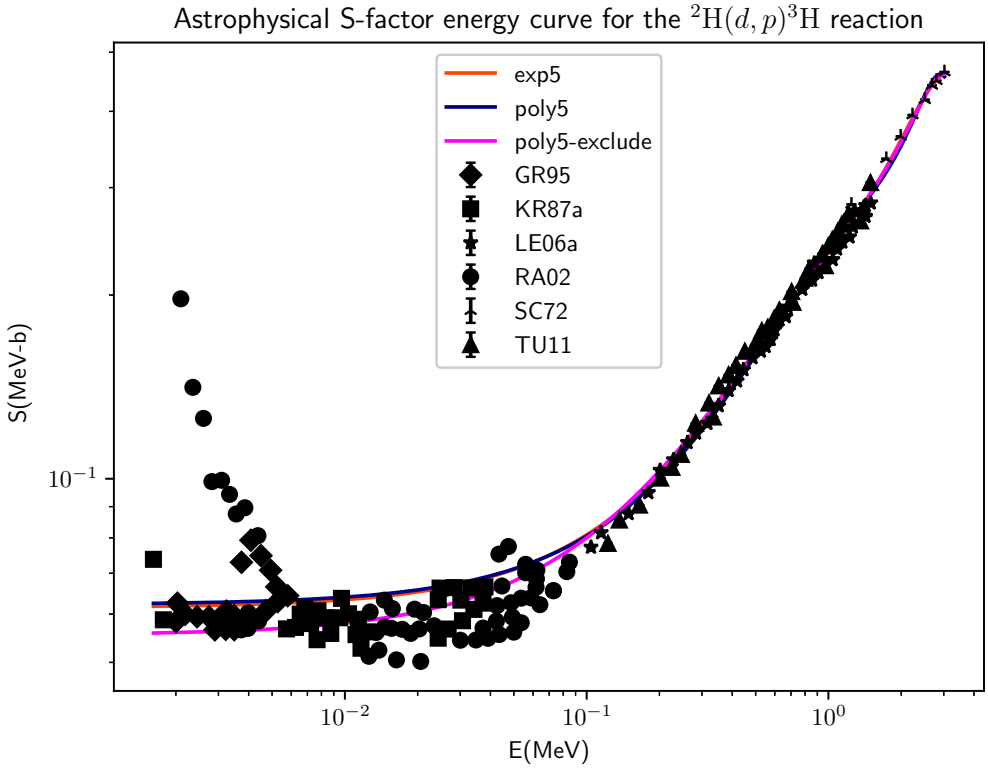
4.1.2 Results and analysis



(a) Polynomial fits.



(b) Exponential fits.



(c) Best fits.

Figure 4.1: Empirical formulas fitted to ^{2}H(d, p)^{3}H reaction S-factor data. In panel a), poly1, poly2, poly3, poly4, and poly5 represent fits to polynomials from 1st to 5th order. Similarly, in panel b), exp1, exp2, exp3, exp4 and exp5 represent exponential fits up to 5th order. Additionally, in panel c), poly5-exclude corresponds to a poly5 fit without data from RA02 and GR95. References to the sources of the black colored experimental points are given in Table A.1. Fitting parameters values are given in Tables C.2 and C.3.

At low-energies as far as 10^{-3} MeV $< E < 10^{-2}$ MeV, an exponential-like damping of the S-factor is observed. In fact, this behavior could explained due to the electron screening effect [25]. In particular, the enhancement factor f for the S-factor is defined as [25]:

$$f = \frac{E}{E + U_e} \exp\left(\frac{\pi \eta U_e}{E}\right), \tag{4.5}$$

where E is the center of mass energy, η is the Sommerfeld parameter and U_e is a parameter that quantifies the degree of enhancement of the S-factor. The sharp increase of the S-factor at low energies is explained by the shielding of the Coulomb potential produced by the electron cloud that surrounds the interacting nuclei [26]. In particular, this dismissal of the strength of the potential reduces the Coluomb barrier. Therefore, as the tunneling probability increases, the cross-section for the reaction also increases.

Additionally, the value of the U_e parameter is usually obtained by fitting. An example of such fitting is found in the graphs of Figure 4.2.

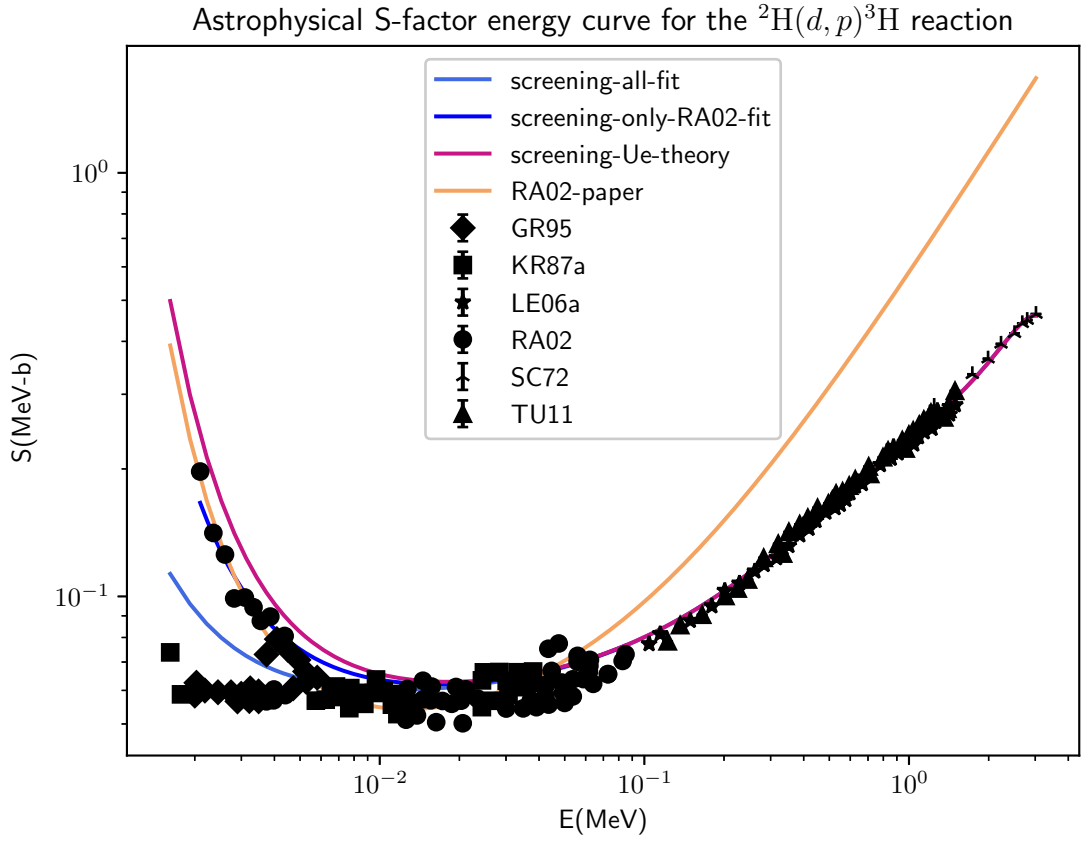
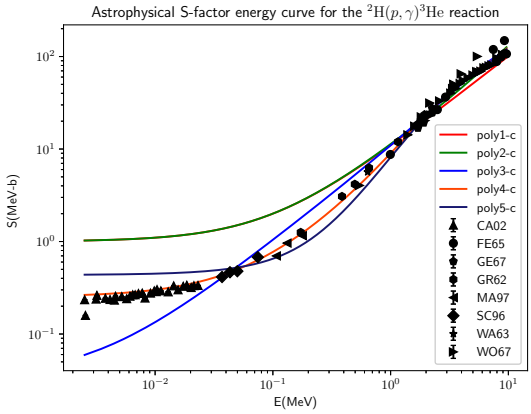
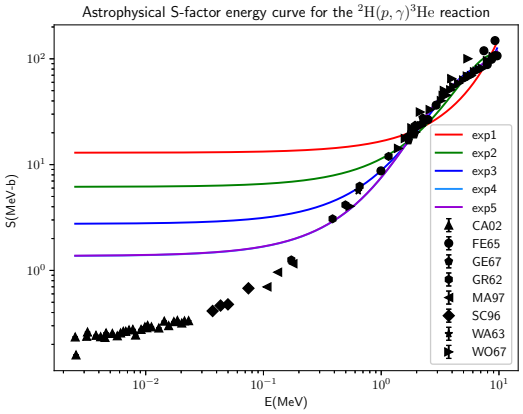


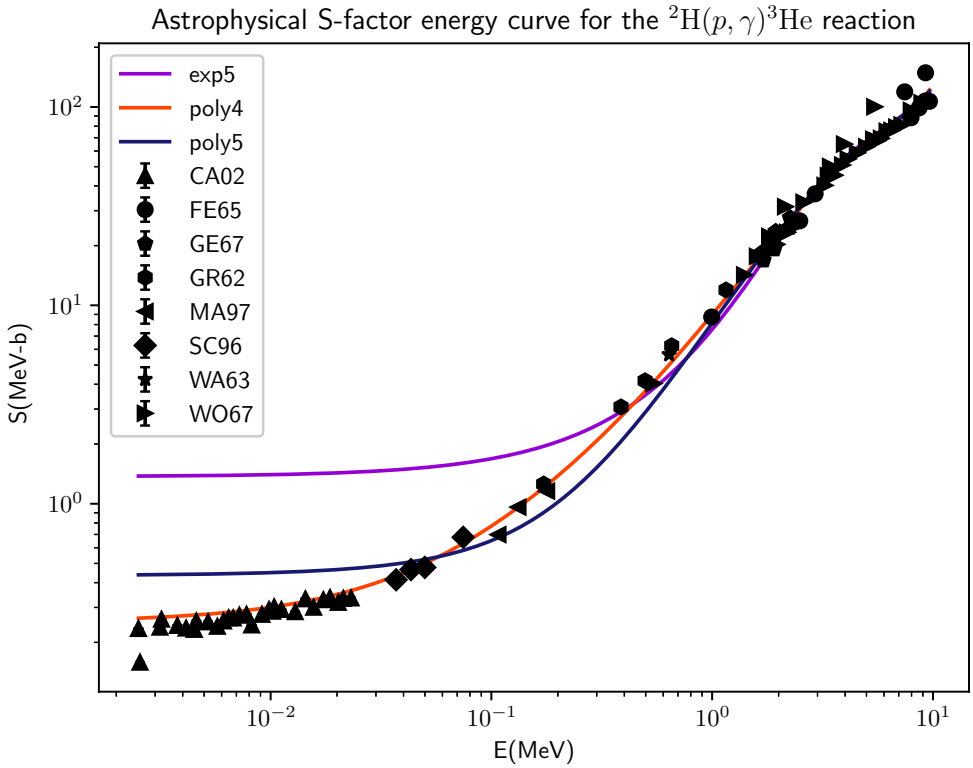
Figure 4.2: Polynomial fits to experimental data with screening effect. The curve labeled as screening-all-fit is obtained by fitting U_e with all data points, screening-only-RA02-fit is obtained only with RA02 data, *screening-Ue-theory* is calculated with U_e fixed to the value given in RA02. The poly5-exclude fit of Figure 4.1 was used as the S-factor estimation without screening of the last three curves. Additionally, the screening-RAO2 curve presents the S-factor prediction made in the RA02 paper. Further details about the fitting parameters and their values are given in Table C.4.



(a) Polynomial fits with constraints.



(b) Exponential fits.



(c) Selected fits.

Figure 4.3: Empirical formulas fitted to the S-factor for the ^{2}H(p,γ)^{3}He reaction. In panels a) and b) polynomial and exponential fits up to fifth order are presented respectively. In particular, the fit parameters used for the graphs in panel a) were constrained. Additionally, in panel c), the best selected fits are visualized. The references to the experimental points are given in Table A.1. The values of the fitting parameters are encountered in Tables C.5 and C.6.

S-factor curve for the low energy regime in Figure 4.3.

Exponential fit does not converge as desired at low-energies.

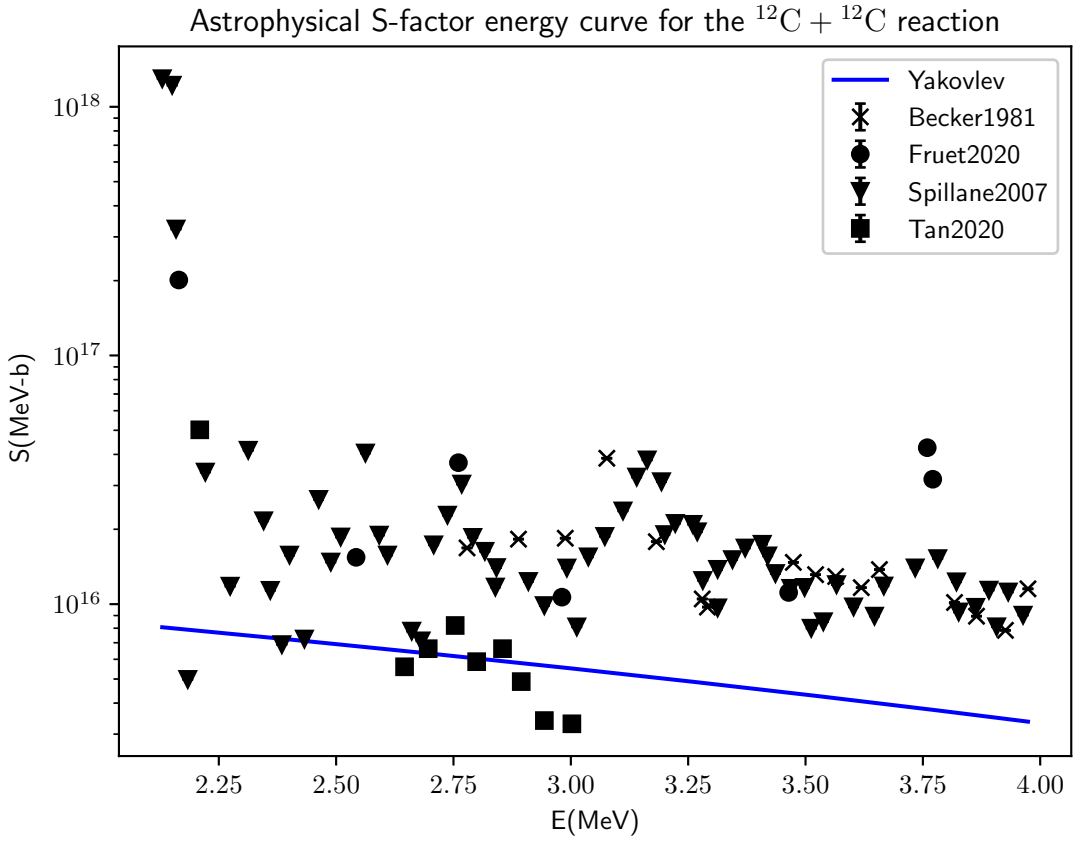


Figure 4.4: Astrophysical S-factor prediction for the $^{12}C + ^{12}C$ reaction as parametrized in the Yakovlev et. al analytical potential model [119]. Experimental points references are presented in Table A.3.

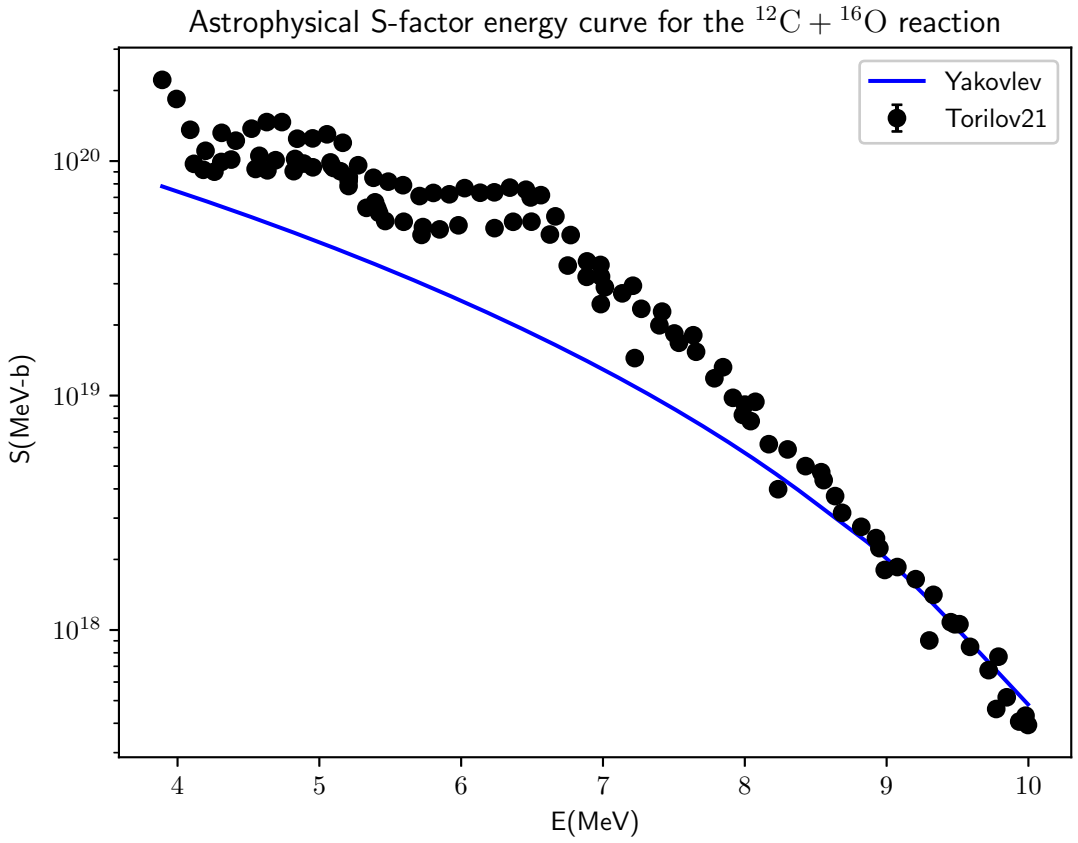
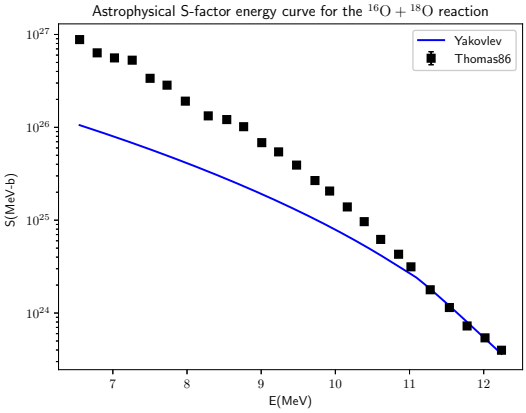
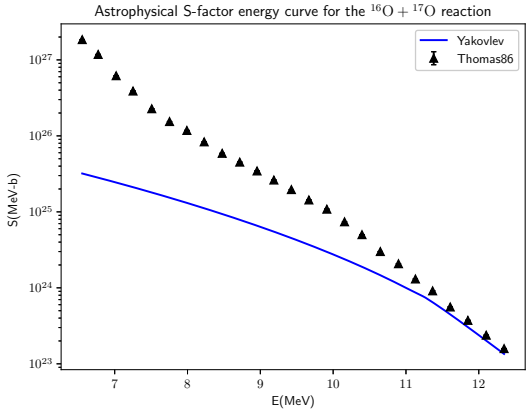


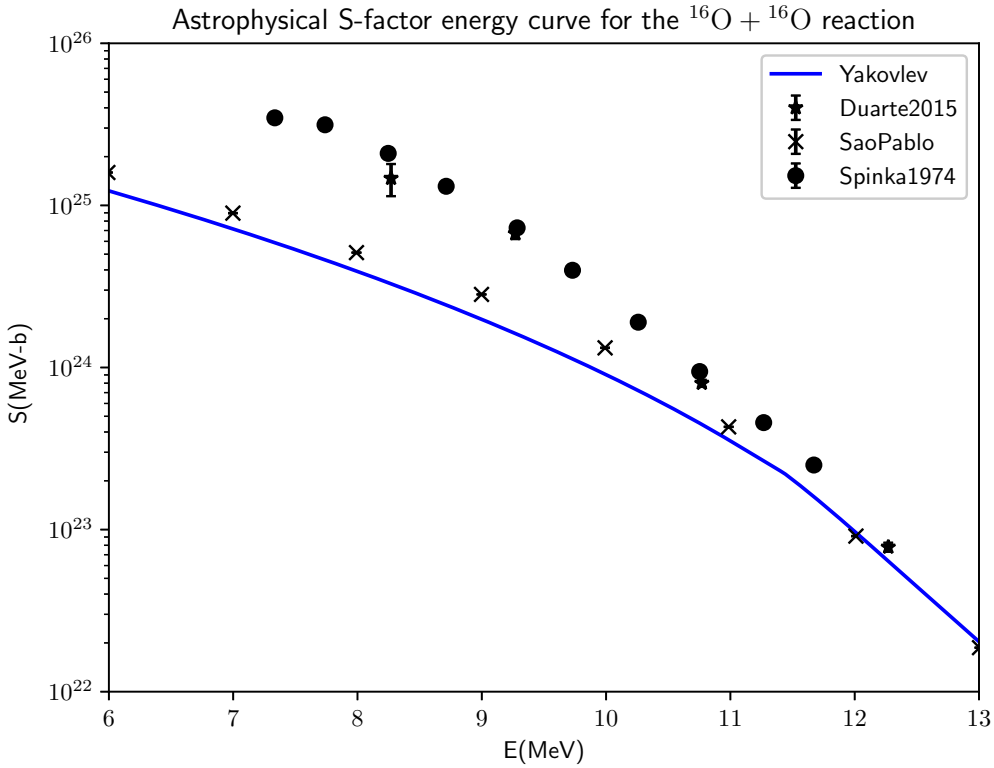
Figure 4.5: Astrophysical S-factor prediction for the $^{12}C + ^{16}O$ reaction as parametrized in the Yakovlev et. al analytical potential model [119]. The reference for the experimental points is given in Table A.3.



(a) $^{16}O + ^{18}O$ reaction.



(b) $^{16}O + ^{17}O$ reaction.



(c) $^{16}O + ^{16}O$ reaction.

Figure 4.6: Potential model prediction for a selection of oxygen fusion reactions. In panels a), b) and c) are presented the Yakovlev et. al prediction for the S-factor of the $^{16}O + ^{18}O$, $^{16}O + ^{17}O$ and $^{16}O + ^{16}O$ reactions respectively. Additionally, in panel c), the *SaoPablo* entry corresponds with the predictions made in [119] which were obtained by using the São Pablo potential model. Experimental data sources are cited in Table A.3.

4.6 4.6c 4.6b 4.6a

4.2 Resonant reactions

It is frequent to find sharp peaks in the S-factor values of some nuclear reactions. The existence of these fluctuations usually suggest the presence of resonant phenomena. In particular, each peak is characterized by additional variables like its height, width and energy center. Then, the non-resonant astrophysical S-factor predictions of section 4.1 shall be modified.

A first apporach towards the description of resonances Breit-Wigner. Single channel approximation.

$^{7}\mathrm{Be}(\mathrm{p},\gamma)^{8}\mathrm{B}$ and $^{13}\mathrm{C}(\mathrm{p},\gamma)^{14}\mathrm{N}$

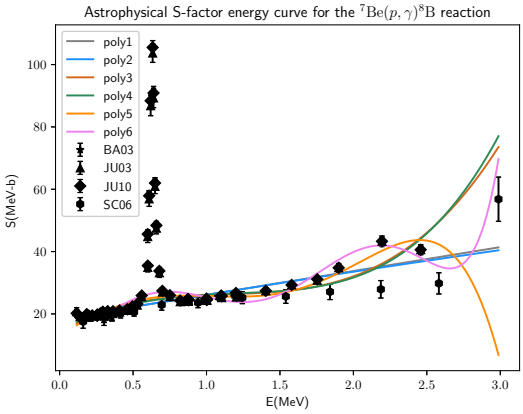
A compilation of additional R-matrix treatment is given by [153].

4.2.1 Calculation considerations

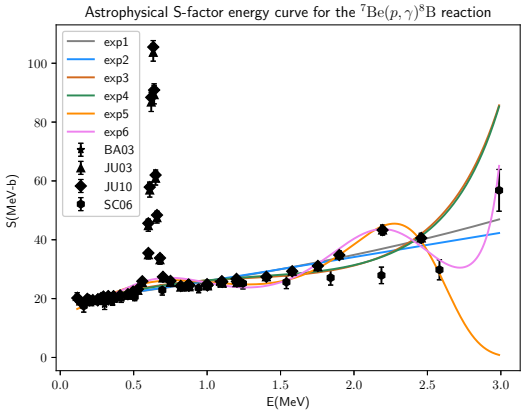
Breit-Wigner empirical formula was used for initial fitting.

4.2.2 Results and analysis

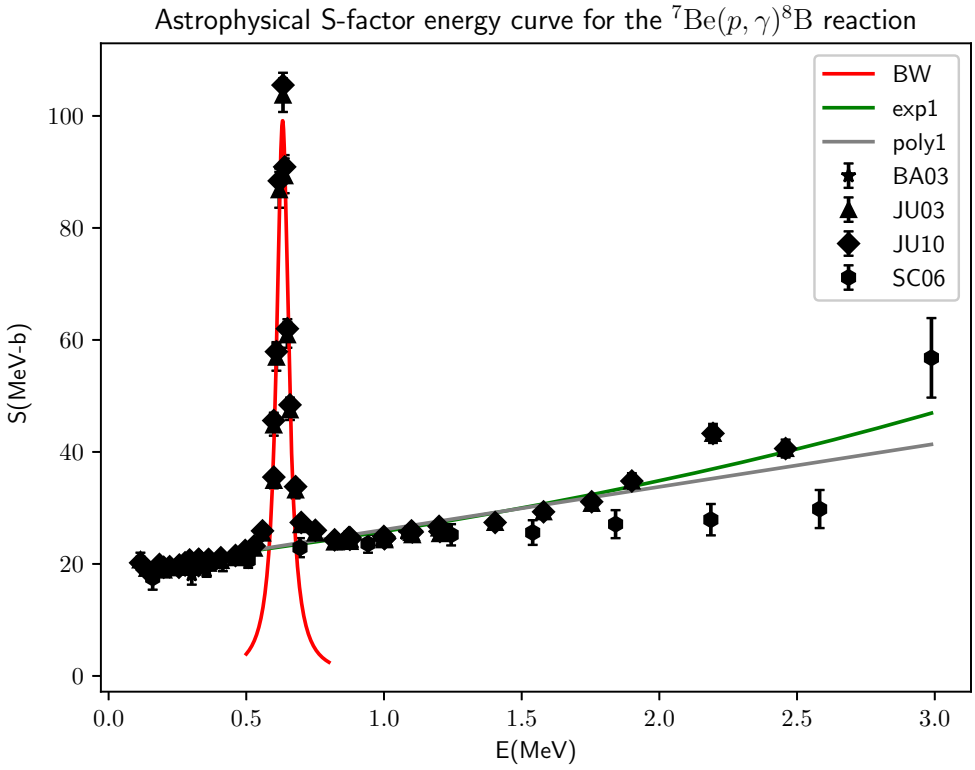
Background estimation with non-resonant fits.



(a) Polynomial fits.



(b) Exponential fits.



(c) Selected fits.

Figure 4.7: Empirical formulas fitted to background of the S-factor for the ^{7}Be(p,γ)^{8}B reaction. In panels a) and b) polynomial and exponential fits up to sixth order are presented respectively. Additionally, in panel c), the most simple and accurate fits, in this case exp1 and poly1, were selected. In addition, the BW labeled curve corresponds to a Breit-Wigner fit for the resonance. The references to the experimental points are given in Table A.2. The values of the fitting parameters are found in Tables C.7, C.8 and C.9.

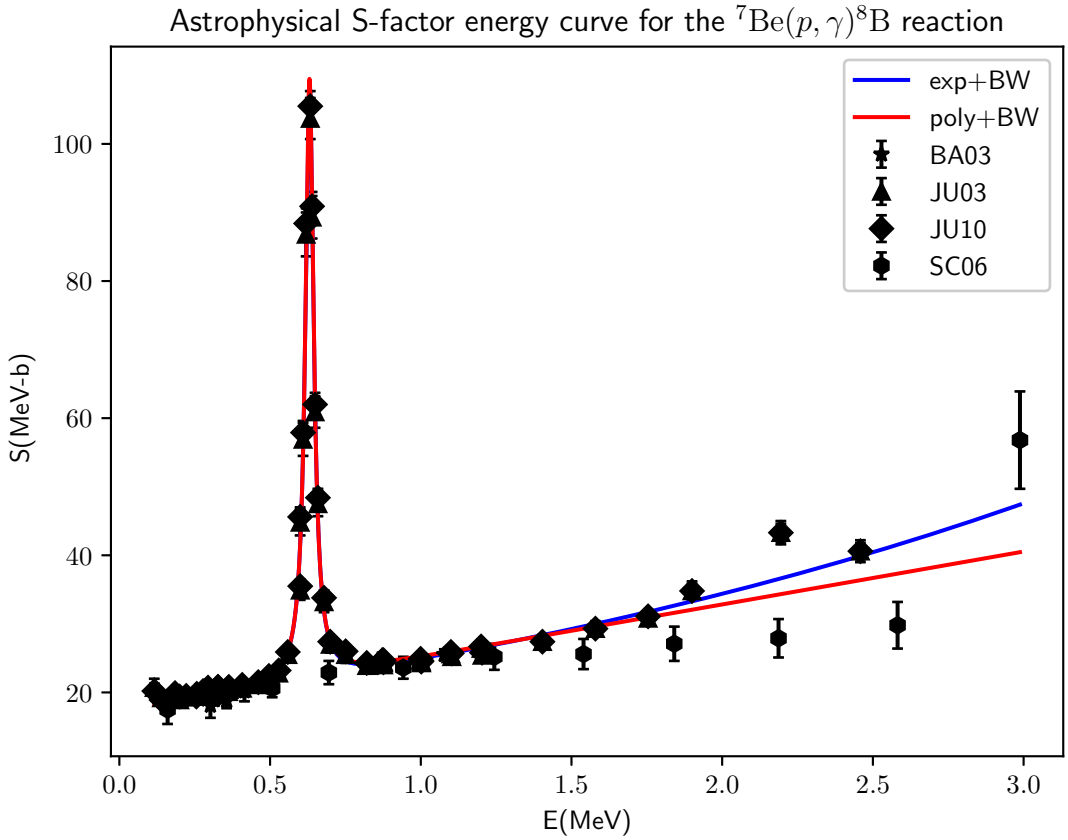


Figure 4.8: Empirical fit for the ^{7}Be(p,γ)^{8}B reaction. In this graph, the resonant contribution, as modeled with a Breit-Wigner, was added to the non-resonant background estimation, which was modeled with first order polynomial and exponential formulas. In addition, fitting parameters are found in Table C.10.

A single resonance with a peak close to $E = 0.7$ MeV is observed in Figure 4.8. Then, in order to model the single resonance, a Breit-Wigner fit was performed.

However, as it is visualized in S-factor dependence, this fit does not account for the entire behavior of the experimental points far from the resonance. Consequently, the theoretical prediction is modified to improve the modeling of the non-resonant part of the S-factor.

Additionally, an increment of the background, namely the non-resonant part of the S-factor, is present.

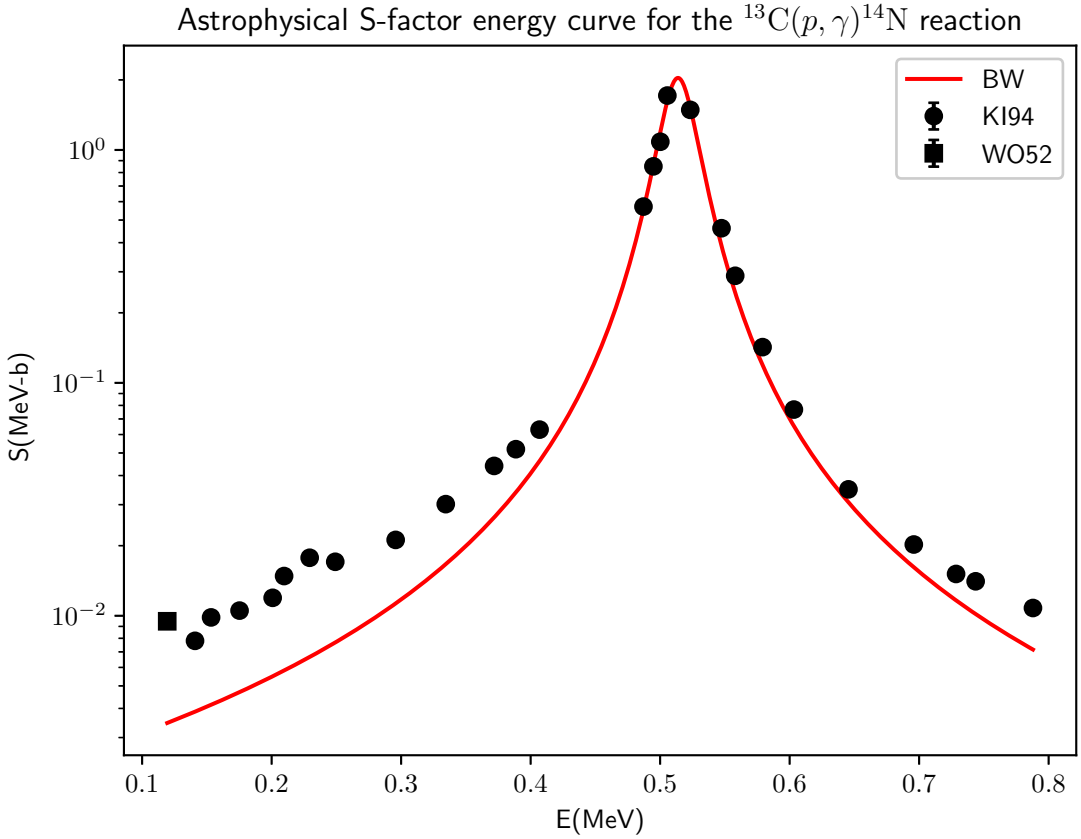
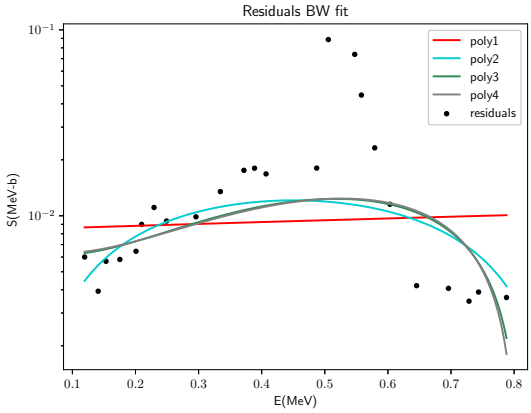


Figure 4.9: Breit-Wigner fit for the S-factor of the resonant $^{13}C(p,\gamma)^{14}N$ reaction. The experimental data points were taken from sources cited in Table A.2. Further details about the fitting parameters and their values are given in Table C.11.

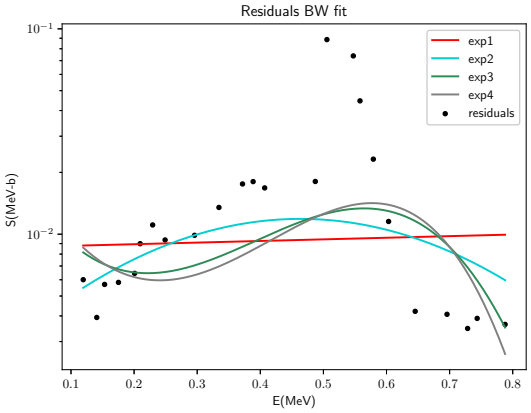
A resonance with a peak close to $E = 0.6$ MeV is observed in the S-factor data presented of Figure 4.9. In order to model this behavior, a Breit-Wigner fit was initially performed.

Despite the global correspondence between the experimental data and the predictions of the fit, the resonant behavior does not entirely explain the shape of the S-factor data. This discrepancy specially occurs far from the resonance peak at low energies. In order to improve the prediction, the non-resonant contribution to the S-factor needs to be included.

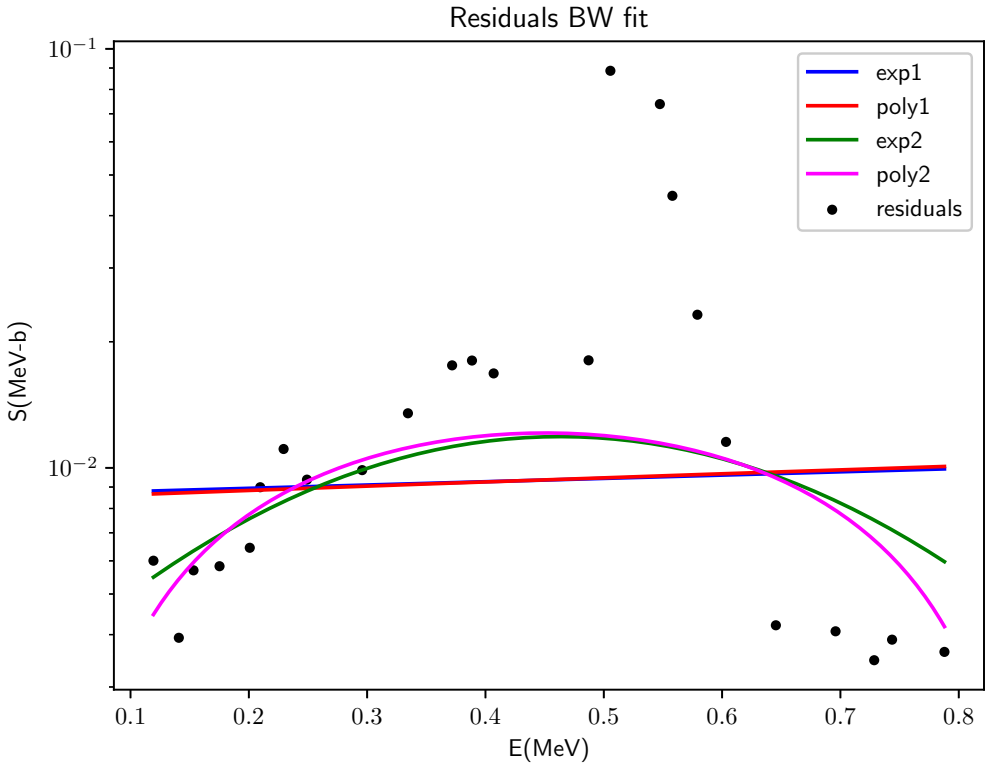
In a first approach, the non-resonant background is modeled empirically. In particular, the polynomial and exponential expansion was used.



(a) Polynomial fits.



(b) Exponential fits.



(c) Selected fits.

Figure 4.10: Empirical formulas fitted to background of the S-factor for the $^{13}C(p,\gamma)^{14}N$ reaction. The background was quantified with the residuals of the Breit-Wigner fit of Figure 4.9. he values of the fitting parameters are found in Tables C.12 and C.13.

The correspondence between the joint resonant and non-resonant prediction with experimental data at low energies improved at low energies. However, at energies above the resonance peak, the fit overestimated the S-factor.

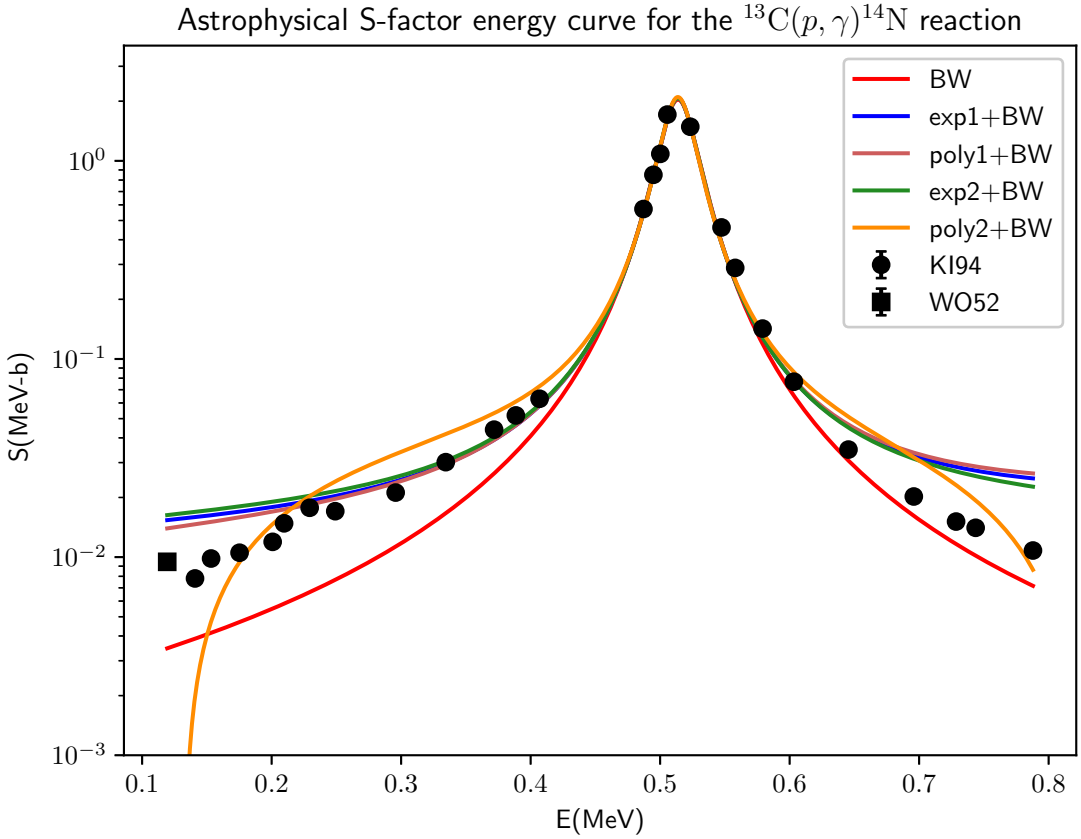


Figure 4.11: Empirical fit for the S-factor of the resonant $^{13}C(p,\gamma)^{14}N$ reaction. The resonant part was estimated with a Breit-Wigner fit added to a non-resonant background, which was fitted with exponential and polynomial with first and second order formulas. All the values of the parameters used are found in Table C.14.

This difference could be explained due to particularities of the physical phenomena underlying the $^{13}C(p,\gamma)^{14}N$ reaction. In fact, the S-factor values presented in Figure 4.9 corresponds to the sum of different channels associated with non-excited and excited states of ^{14}N [154]. This means that the theoretical prediction should consider the transitions to all possible states of the reactants and product nuclei.
The $^{12}C + ^{12}C$ channel have various resonances. These resonances could be explained from the Trojan Horse method or other alternative microscopical methods.

Chapter 5

Conclusions

Astrophysical S-factors were calculated for the selected reactions and compared with available experimental data.

Nuclear physics of stars. Christian Iliadis.

Cauldrons in the cosmos. Claus Rolfs.

Hyde and Basdevant Nuclear physics.

Appendix A

Literature selected data

A.1 General data of nuclei

In this section general data about the structure of the nuclei will be presented.
EXFOR [155].
Japanese database [156].

A.1.1 Selected constants

NIST selected constants and conversion factors to convenient units.

The units used for calculations are those suitable for calculations of astrophysical S-factors. In particular, the unit of energy is given in mega-electronvolts (MeV), and the distances between nuclei are given in fentometers (fm), and the cross sections in barns (1b = 10^{-28}cm). Therefore, various fundamental constant are converted to consistent units with respect to the mentioned convention as shown in the next table.

Some constants to be considered: c, h, $\hbar$, m_e, m_p, m_n.

In the units to be used for nuclear physics calculations: $4\pi\epsilon_0 = 1$. So, the fine structure constant is expressed as:

$$\alpha = \frac{e^2}{\hbar c}. \tag{A.1}$$

Therefore, the elementary charge is given by:

$$e = \sqrt{\alpha\hbar c} \approx \sqrt{1.41...}\sqrt{\text{MeV fm}}. \tag{A.2}$$

Masses can be expressed in terms of MeV/c^2 or MeV fm^{-2} s^2 depending on the context.

A.1.2 Nuclei structure data

atomic, massic, mass excess, spin, charge, data. L^π.

A.2 Astrophysical S-factor data

In this section, the reference to the experimental data on astrophysical S-factors for the selected reactions will be presented. In particular, the II database was widely used for reactions with $A < 10$. On the other hand, for reactions with $A > 10$, more specific references were used to obtain the experimental data.

Additional, light heavy experimental data pd reaction [157] and 2H proton capture c[158] and He3 photo-disintegration [159] with [160]

A.2.1 Nacre II database

The experimental data for a wide selection of radiative capture and exchange reactions at low energies is found in the Nacre II database [154]. This database serves as a compilation of data obtained form various experiments for the relevant reactions. In addition, in this paper a potential model calculation for each reaction is also included.

In the following tables, the references to the papers form which experimental data was obtained form this work will be presented.

Light nuclei reactions

Name	Reference	Reaction
GR85	[161]	$^{2}\mathrm{H(d,p)^{3}H}$
KR87a	[162]	
LE06a	[163]	
RA02	[25]	
SC72	[164]	
TU11	[165]	
CA02	[166]	$^{2}\mathrm{H(p,\gamma)^{3}He}$
FE65	[167]	
GE67	[168]	
GR62	[169]	
MA97	[170]	
SC96	[171]	
WA63	[160]	
WO67	[172]	

Table A.1: Experimental data references for a selection of non-resonant light heavy nuclei reactions. This table includes data corresponding to the $^{2}\mathrm{H(d,p)^{3}H}$ and $^{2}\mathrm{H(p,\gamma)^{3}He}$ reactions.

Resonant reactions

Name	Reference	Reaction
BA03	[173]	$^{7}\mathrm{Be(p,\gamma)^{8}B}$
JU03	[174]	
JU10	[175]	
SC06	[176]	
KI94	[177]	$^{13}\mathrm{C(p,\gamma)^{14}N}$
WO52	[178]	

Table A.2: Experimental data references for a selection of resonant reactions. This table includes data corresponding to the $^{7}\mathrm{Be(p,\gamma)^{8}B}$ and $^{13}\mathrm{C(p,\gamma)^{14}N}$ reactions.

A.2.2 Middle heavy nuclei data

Selected reaction reference table for the $^{12}\mathrm{C}+{}^{12}\mathrm{C}$, $^{12}\mathrm{C}+{}^{16}\mathrm{O}$, $^{16}\mathrm{O}+{}^{16}\mathrm{O}$, $^{13}\mathrm{C}+{}^{13}\mathrm{C}$ reactions.
$^{12}\mathrm{C}+{}^{12}\mathrm{C}$ reaction.

Name	Reference	Reaction
Becker1981	[179]	$^{12}C + ^{12}C$
Fruet2020	[180]	
Spillane2007	[181]	
Tan2002	[182]	
Torilov21	[48]	$^{12}C + ^{16}O$
Thomas86	[45]	$^{16}O + ^{18}O$
		$^{16}O + ^{17}O$
Duarte2015	[43]	$^{16}O + ^{16}O$
Spinka1974	[183]	

Table A.3: Experimental data citations for a selection of oxygen and carbon fusion reactions.

A.3 Resonances and transitions

Resonant specific data will be presented. In particular, for those reactions with the aviable information, the experimental peak as well as the reaction peak will be detailed. Additionally, with special observance on the radiative capture reactions, the transitions will be specified.
Data on the resonant 7Be + p and experimental methods [184].

A.3.1 Resonance data

Selection reaction reference list.

A.3.2 Transitions data

Transition type data, energy levels, energy peak and widths.

A.4 Fitting parameters

The fitting parameters in a selected list of articles will be presented. In particular, this section distinguish between specific model parameters, like empirical, potential or microscopical models, and R-matrix fitting, whose special calculation considerations will be detailed.

A.4.1 Specific model parameters

Tables of models and parameters, with uncertainties.

A.4.2 R-matrix parameters

Tables of parameters that were chosen for the selected reactions

Appendix B

Special functions

In this section will be encountered special functions to be used in scattering theory and solution of analytical equations.

B.1 Bessel functions

Differential equation, solutions, 1st and 2nd kind and some useful properties. There are standard and spherical Bessel functions.

The spherical functions are solutions for the differential equation:

$$\frac{d^2x}{d\rho^2} + 2\rho\frac{dx}{d\rho} + (\rho^2 - l(l+1))x = 0. \tag{B.1}$$

In particular, the solutions $J_l(\rho)$ and $Y_l(\rho)$ are called the Bessel and Von-Neumann solutions. One difference between these solutions is that $J_l(\rho)$ is well defined while $Y_l(\rho)$ has a pole at that $\rho = 0$.

In addition, the asymptotic behavior when $\rho \to \infty$ is different for each function as shown:

$$J_l(\rho) \to \sqrt{\frac{2}{\pi\rho}} \cos\left(\rho - \frac{\pi}{4} - \frac{l\pi}{2}\right). \tag{B.2}$$

and

$$Y_l(\rho) \to \sqrt{\frac{2}{\pi\rho}} \sin\left(\rho - \frac{\pi}{4} - \frac{l\pi}{2}\right). \tag{B.3}$$

B.2 Coulomb functions

Differential equations, solutions and more properties.

$$\frac{d^2x}{d\rho^2} + (\rho^2 - 2\eta\rho - l(l+1))x = 0. \tag{B.4}$$

There are two solutions for this equations. In the context of scattering theory, the solutions $F_{l\eta}(\rho)$ and $G_{l\eta}(\rho)$ are analogous to the $J_l(\rho)$ and $Y_l(\rho)$ solutions of the Bessel differential equation respectively.

The formulas are connected as [185].

$$G_{l\eta} = \frac{F_{l\eta} - iF_{-l\eta}}{2i}. \tag{B.5}$$

In a similar way than the Bessel functions, the Coulomb functions have harmonic like asymptotic behavior. In particular, $F_{l\eta} \to \sin\theta_{l\eta}$ and $G_{l\eta} \to \cos\theta_{l\eta}$ with $\theta_{l\eta}$ defined as :

$$\theta_{l\eta}(\rho) = \rho - l\frac{\pi}{2} - \eta\ln(2\rho) + \arg\Gamma(l+1+i\eta). \tag{B.6}$$

B.3 Additional selected functions

Hypergeometric equations and connection with coulomb functions with implementation.

Spherical harmonics and Legendre polynomials for the expansions used in scattering theory. Hyperspherical harmonics

B.4 Clebsch-Gordan coefficients

Motivation, definition and some computations. Generalization to further spins and couplings that are useful for determining effects like the spin-orbit coupling.
The total angular momentum and change of basis.

$$J = L + S \tag{B.7}$$

.
Tensor products.

$$a \otimes b. \tag{B.8}$$

$$a \oplus b. \tag{B.9}$$

And the Wigner notation for the Clebsh-Gordan coefficients.

$$\begin{pmatrix} s & l & I_x \\ j_s & j & J \end{pmatrix}. \tag{B.10}$$

B.5 Microscopic model functions

Those relevant microscopic model methods. Specially, those that account for cluster model and effective field theory models.

Hamiltonians and Lagrangians of related field theories.

Appendix C

Fitting

This section is about fitting considerations on the different approaches used to calculate the astrophysical S-factor.

C.1 Calculation procedures

Least square minimization of the quantity shown in equation C.1.

$$\chi^2 = \sum_{k=1}^{N} \frac{(x_k - \bar{x})^2}{\sigma_k^2}, \tag{C.1}$$

where k is an index running through all N of the sample points, x_k is the value, σ_k is the error of each point and $\bar{x}$ corresponds to the average of the value taken from all points.

There are two process depending if the optimization is bounded or unbounded.

C.1.1 Unconstrained fitting

Leavenberg-Marquardt algorithms [186] and more recently [187].

C.1.2 Constrained fitting

Trust region reflective algorithm [188] and more theory [189].

C.2 Empirical formulas fitting

Parameter list with uncertainty for its respective formula.

Units for the fitting parameters related with exponential and polynomial fits.

Label	g_0	g_1	g_2	g_3	g_4	g_5	g_6
poly	MeV b	b	MeV^{-1} b	MeV^{-2} b	MeV^{-3} b	MeV^{-4} b	MeV^{-5} b
exp		MeV^{-1}	MeV^{-2}	MeV^{-3}	MeV^{-4}	MeV^{-5}	MeV^{-6}

Table C.1: Units of the exponential and polynomial parameters.

Polynomial. $^2\mathrm{H(d,p)}^3\mathrm{H}$ reaction.

Label	g_0	g_1	g_2	g_3	g_4	g_5
poly1	0.0680 ± 0.0017	0.152 ± 0.0025				
poly2	0.0627 ± 0.0016	0.193 ± 0.0052	-0.0205 ± 0.0023			
poly3	0.0613 ± 0.0016	0.218 ± 0.011	-0.0523 ± 0.013	0.00847 ± 0.0034		
poly4	0.0615	0.212	-0.0401	0.00128	1.000	
poly5	0.0622 ± 0.0018	0.173 ± 0.032	0.116 ± 0.094	-0.189 ± 0.097	0.0886 ± 0.040	-0.0133 ± 0.0058
poly5-exclude	0.0554 ± 0.0013	0.254 ± 0.015	-0.0827 ± 0.041	-0.00712 ± 0.042	0.0197 ± 0.017	-0.00417 ± 0.0024

Table C.2: Fitting parameters of the polynomial fits, presented in Figures 4.1a and 4.1c, of the $^2\mathrm{H}(\mathrm{d},\mathrm{p})^3\mathrm{H}$ reaction.

Exponential

Label	g_0	g_1	g_2	g_3	g_4	g_5
exp1	0.0929 ± 0.003	0.622 ± 0.019				
exp2	0.0724 ± 0.0018	1.397 ± 0.039	-0.271 ± 0.013			
exp3	0.066 ± 0.0016	2.028 ± 0.075	-0.888 ± 0.066	0.145 ± 0.015		
exp4	0.0674	1.847	-0.623	0.0191	1.000	
exp5	-2.789 ± 0.026	3.011 ± 0.22	-2.818 ± 0.51	1.495 ± 0.46	-0.384 ± 0.17	0.459 ± 0.023

Table C.3: Fitting parameters of the exponential fits, presented in Figure 4.1b, of the $^2\mathrm{H}(\mathrm{d},\mathrm{p})^3\mathrm{H}$ reaction.

Screening with poly5-exclude

Label	Comment	U_e(eV)
screening-all-fit	Fitting	100.0 ± 8.6
screening-only-RA02-fit	Fitting without RA02 data included	230.7 ± 9.2
screening-Ue-theory	Calculation with RA02 U_e value	309 ± 12 [25]
RA02-paper	Prediction RA02 paper	

Table C.4: Screening effect parameter U_e values related to $^2\mathrm{H}(\mathrm{d},\mathrm{p})^3\mathrm{H}$ reaction fits presented in Figure 4.2. In the RA02-paper curve a poly1 for background estimation was used with parameters $g_0 = 0.0043 \pm 0.0001$ MeV b and $g_1 = 0.54 \pm 0.05$ b [25].

Polynomial.

Label	g_0	g_1	g_2	g_3	g_4	g_5
poly1-c	1.0 ± 1.5	10.00 ± 0.43				
poly2-c	1.0 ± 1.2	10.00 ± 0.93	0.309 ± 0.11			
poly3-c	0.0342 ± 1.1	10.0 ± 1.8	1.011 ± 0.55	-0.0839 ± 0.043		
poly4-c	0.253 ± 1.1	4.712 ± 3.30	4.803 ± 1.9	-0.830 ± 0.34	0.0432 ± 0.019	
poly5-c	0.434 ± 1.2	1.389 ± 5.96	7.980 ± 5.1	-1.829 ± 1.5	0.169 ± 0.19	-0.00547 ± 0.0081

Table C.5: Fitting parameters polynomial fits, shown in Figure 4.3a, ^{2}H(p, γ)^{3}He reaction.

Exponential

Label	g_0	g_1	g_2	g_3	g_4	g_5
exp1	12.958 ± 1.4	0.250 ± 0.014				
exp2	6.165 ± 0.86	0.649 ± 0.047	-0.0367 ± 0.038			
exp3	2.754 ± 0.64	1.334 ± 0.14	-0.181 ± 0.025	0.00865 ± 0.0014		
exp4	0.311 ± 0.45	2.116 ± 0.39	-0.447 ± 0.12	0.0439 ± 0.014	-0.00159 ± 0.00063	
exp5	0.315 ± 0.62	2.109 ± 0.73	-0.444 ± 0.33	0.0431 ± 0.067	-0.00151 ± 0.0064	-0.000294 ± 0.00023

Table C.6: Fitting parameters exponential fits, shown in Figure 4.3b, related to the ^{2}H(p, γ)^{3}He reaction.

Polynomial. ^{7}Be(p, γ)^{8}B reaction. Non-resonant background.

Label	g_0	g_1	g_2	g_3	g_4	g_5	g_6
poly1	18.429 ± 0.86	7.668 ± 1.1					
poly2	18.316 ± 1.3	8.042 ± 3.3	-0.217 ± 1.8				
poly3	13.868 ± 2.3	29.490 ± 10.0	-24.403 ± 10.8	7.101 ± 3.1			
poly4	15.075	22.690	-13.835	1.106	0.000		
poly5	13.219 ± 5.4	27.594 ± 35.8	-0.187 ± 79.8	-35.841 ± 78.3	26.055 ± 34.3	-5.072 ± 5.4	
poly6	27.181 ± 7.7	-103.057 ± 63.1	419.070 ± 185.7	-631.656 ± 251.3	435.745 ± 167.9	-138.269 ± 53.8	16.382 ± 6.6

Table C.7: Parameters polynomial fits, included in Figure 4.7a, corresponding to ^{7}Be(p, γ)^{8}B reaction.

Exponential

Label	g_0	g_1	g_2	g_3	g_4	g_5	g_6
exp1	19.091 ± 0.71	0.301 ± 0.042					
exp2	18.731 ± 1.1	0.356 ± 0.13	-0.0278 ± 0.060				
exp3	16.162 ± 1.5	1.024 ± 0.36	-0.734 ± 0.36	0.194 ± 0.096			
exp4	16.985	0.770	-0.388	0.0261	0.000		
exp5	2.645 ± 0.29	1.355 ± 1.9	0.295 ± 4.3	-2.425 ± 4.2	1.720 ± 1.9	-0.344 ± 0.30	
exp6	3.071 ± 0.36	-2.499 ± 2.7	12.451 ± 7.5	-19.720 ± 9.6	13.799 ± 6.1	-4.382 ± 1.9	0.516 ± 0.22

Table C.8: Parameters exponential fits, included in Figure 4.7b, associated with the $^{7}\mathrm{Be}(\mathrm{p},\gamma)^{8}\mathrm{B}$ reaction.

BW $^{7}\mathrm{Be}(\mathrm{p},\gamma)^{8}\mathrm{B}$

Label	S_r(MeV b)	E_r(MeV)	Γ_r(MeV)
BW	99.153 ± 4.9	0.632 ± 0.0010	0.0535 ± 0.0034

Table C.9: Fitting parameters to the Breit-Wigner function, shown in Figure 4.7c, for the $^{7}\mathrm{Be}(\mathrm{p},\gamma)^{8}\mathrm{B}$ reaction.

Composite $^{7}\mathrm{Be}(\mathrm{p},\gamma)^{8}\mathrm{B}$

Label	S_r(MeV b)	E_r(MeV)	Γ_r(MeV)	c_r(MeV^2)	g_0	g_1
exp + BW	87.097 ± 2.2	0.631 ± 0.00036	0.0335 ± 0.00095		17.935 ± 0.13	0.325 ± 0.0077
poly + BW	21.227	0.631 ± 0.00062	0.0331	0.00113	17.370 ± 0.20	7.725 ± 0.27

Table C.10: Fitting parameters for composite resonant and non-resonant behavior fits, as visualized in Figure 4.8, for the $^{7}\mathrm{Be}(\mathrm{p},\gamma)^{8}\mathrm{B}$ reaction.

BW $^{13}\mathrm{C}(\mathrm{p},\gamma)^{14}\mathrm{N}$

Label	S_r(MeV b)	E_r(MeV)	Γ_r(MeV)
BW	2.040 ± 0.059	0.514 ± 0.00026	0.0325 ± 0.0013

Table C.11: Fitting parameters Breit-Wigner fits, included in Figure 4.9, related to the $^{13}\mathrm{C}(\mathrm{p},\gamma)^{14}\mathrm{N}$ reaction.

Residuals polynomial fit $^{13}\mathrm{C}(\mathrm{p},\gamma)^{14}\mathrm{N}$ reaction.

Label	g_0	g_1	g_2	g_3	g_4
poly1	0.00841 ± 0.016	0.00211 ± 0.033			
poly2	-0.00204 ± 0.032	0.0628 ± 0.17	-0.0697 ± 0.19		
poly3	0.00694 ± 0.076	-0.0193 ± 0.65	0.135 ± 1.6	-0.150 ± 1.1	
poly4	0.00678	-0.0134	0.0943	-0.0606	1.000

Table C.12: Fitting parameters polynomial fit residuals, as visible in Figure 4.10a, for the $^{13}C(p,\gamma)^{14}N$ reaction.

Residuals exponential fit $^{13}C(p,\gamma)^{14}N$ reaction.

Label	g_0	g_1	g_2	g_3	g_4
exp1	0.00862 ± 0.015	0.181 ± 3.6			
exp2	0.00292 ± 0.013	6.049 ± 21.3	-6.526 ± 23.9		
exp3	0.0238 ± 0.23	-13.564 ± 83.3	42.626 ± 205.1	-36.166 ± 153.3	
exp4	0.0306	-15.084	39.610	-17.343	0.000

Table C.13: Fitting parameters exponential fit t residuals, as shown in Figure 4.10b, for the $^{13}C(p,\gamma)^{14}N$ reaction.

Composite $^{13}C(p,\gamma)^{14}N$

Label	S_r	E_r	Γ_r	c_r	g_0	g_1	g_2
exp1 + BW	2.056 ± 0.062	0.514 ± 0.00025	0.0314 ± 0.0014		0.0113 ± 0.014	0.612 ± 2.4	
poly1 + BW	2.057	0.514 ± 0.00026	0.0314	0.000247 ± 0.0014	0.00910 ± 0.017	0.0135 ± 0.037	
exp2 + BW	2.057 ± 0.063	0.514 ± 0.00026	0.0314 ± 0.0015		0.0117 ± 0.033	1.0 ± 15.1	-0.770 ± 16.3
poly2 + BW	2.041	0.514 ± 0.00025	0.031 ± 0.0015	0.000236	-0.037 ± 0.039	0.294 ± 0.22	-0.310 ± 0.24

Table C.14: Fitting parameters composite fits, included in Figure 4.11, corresponding to the $^{13}C(p,\gamma)^{14}N$ reaction.

C.3 Free parameters fitting on potential models

Parameter list, uncertainty and its respective formula.
[190] Sao Pablo potential.

[191] Woods-Saxon potential.

C.4 Microscopic model fitting

Parameter list, uncertainty and its respective formula.

[192]

C.5 R-matrix fitting

Parameter list, uncertainty and its respective formula. Widths and channels.

Reaction	E_R(MeV)	Γ(MeV)	References
1	0.504	0.102	REF1
4	0.607	0.304	REF2

Table C.15: A new Table

[193] [194] [195]

Appendix D

Numerical integration and differential equation solving

In this section will be introduced the generalities of the numerical solution of integrals and differential equation that were used throughout the document. In particular, a special subsection on the numerical solution for the Schroödinger equation for scattering phenomena will be presented.

D.1 Integration of selected potentials

WKB numerical implementation based on the Gaussian quadrature algorithm.

D.2 Numerical solution of the Schrödinger equation

The numerical solution of the Schrödinger equation is found to be useful for the approaches where it is not possible to find a solution for the problem in closed form, mainly analytical solutions.
[196]
Coupled channels [197].

D.2.1 Main approach

The different methods to be solved the Schroödinger equation and overall differential equation solving strategy.

D.2.2 Implementation of the potential functions

Different potential considerations.

D.2.3 Boundary conditions implementation

Expected boundary conditions at $r \to \infty$ and their numerical implementation.

Appendix E

Computer codes implementation

In this section is going to be presented the aspects related with the `sfactors` python module.

E.1 Structure of the computer program

The full tree with the files with explanation of the detailed packages.

E.2 User manual

In this section the user manual should be presented.

E.2.1 Installation

In this section a full installation sequence will be presented

E.2.2 Plotting

Plotting of S-factors.

E.2.3 Empirical fitting

Empirical fitting based on predetermined and custom functions.

E.2.4 Specific model fitting

Model fitting.

E.2.5 Model testing

Different tests of the program code.

E.3 Documentation

E.3.1 Databases

E.3.2 Non resonant

E.3.3 Resonant

E.3.4 Plots

E.3.5 Reconstructed Plots

E.3.6 Solver

E.3.7 Utils

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