Theoretical calculation of nuclear reactions of interest for Big Bang Nucleosynthesis

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# List of Abbreviations

| Abbreviation | Description |
|--------------|-------------|
| $\chi$EFT   | Chiral Effective Field Theory |
| ANC         | Asymptotic Normalization Coefficient |
| AV18        | Argonne $v_{18}$ (potential) |
| BBN         | Big Bang Nucleosynthesis |
| BR          | Branching Ratio |
| BSM         | Beyond Standard Model |
| CD-B2k      | Charge Dependent-Bonn2000 (potential) |
| CFF         | Cluster Form Factor |
| c.m.        | Center of Mass |
| FES         | First Excited State |
| GFMC        | Green’s Function Monte Carlo |
| GS          | Ground State |
| HH          | Hyperspherical Harmonic |
| LEC         | Low-Energy Constant |
| LO          | Leading-Order |
| N2LO/NNLO   | Next-to-Next-to-Leading-Order |
| N3LO        | Next-to-Next-to-Next-to-Leading-Order |
| N4LO        | Next-to-Next-to-Next-to-Next-to-Leading-Order |
| NCSM        | No-Core-Shell-Model |
| NLO         | Next-to-Leading-Order |
| NN          | Nucleon-Nucleon |
| NSHH        | Non-Symmetrized Hyperspherical Harmonic |
| QCD         | Quantum Chromodynamics |
| RGM         | Resonanting Group Model |
| SBBN        | Standard Big Bang Nucleosynthesis |
| SM          | Standard Model |
| SRG         | Similarity Renormalization Group |
| TC          | Transformation Coefficient |
| UIX         | Urbana IX (three-body potential) |
Contents

1 Introduction .............................. 1
  1.1 The $\alpha + d \rightarrow ^6$Li $+ \gamma$ reaction ......................... 2
  1.2 The $p + ^6$Li $\rightarrow ^7$Be $+ \gamma$ reaction .......................... 5

2 The Hyperspherical Harmonic method for bound states .......................... 7
  2.1 Jacobi coordinates and Hyperspherical variables .......................... 7
  2.2 Hyperspherical Harmonic Functions ........................................ 9
  2.3 The Hyperspherical Harmonic expansion .................................... 14
    2.3.1 Orthogonalization of the basis ..................................... 15
  2.4 The variational wave function ............................................. 18
    2.4.1 Norm and kinetic matrix elements .................................. 19
    2.4.2 Potential matrix element ........................................... 19
  2.5 Technical details of the calculation ...................................... 21

3 The $^6$Li ground state within the Hyperspherical Harmonic basis .............. 25
  3.1 The nuclear potential ..................................................... 25
  3.2 Selection of the states .................................................... 27
  3.3 Results for the $^6$Li ground state ....................................... 29
    3.3.1 Convergence of the HH expansion ................................... 29
    3.3.2 Electromagnetic static properties ................................... 36
    3.3.3 Comparison with literature ......................................... 44

4 The $^6$Li Asymptotic Normalization Coefficient .................................. 45
  4.1 The deuteron and the $\alpha$-particle wave functions ...................... 45
  4.2 The $\alpha + d$ cluster form factor ...................................... 47
    4.2.1 Results for the $\alpha + d$ cluster form factor and ANCs .......... 50
  4.3 Equation for the cluster form factor ..................................... 56
    4.3.1 The projection of the asymptotic states .............................. 57
    4.3.2 Calculation of the source term .................................... 59
  4.4 Results ................................................................. 61

5 The $p + ^6$Li$\rightarrow ^7$Be+$\gamma$ radiative capture reaction .......... 69
  5.1 Theoretical formalism ..................................................... 69
  5.2 The $p + ^6$Li potential model .......................................... 71
  5.3 Results ................................................................. 73
    5.3.1 The astrophysical $S$-factor ....................................... 74
    5.3.2 Angular distribution of photons .................................... 76
    5.3.3 The "He"-resonance ................................................ 79

6 Conclusions ................................................. 83
Chapter 1

Introduction

Big Bang Nucleosynthesis (BBN) predicts the abundances of the light elements formed during the earliest time of the Universe from a fraction of a second to hundreds of seconds. By considering the physics of the Standard Model (SM), BBN is able to predict the abundances of $d$, $^3$He, $^4$He and $^7$Li without free parameters. This theory, which is named Standard BBN (SBBN), obtains a good overall agreement with the primordial abundances inferred from astrophysical observations. The agreement with the data for various nuclear species confirms SBBN strength and self-consistency, making it one of the most important direct cosmological test supporting the hot Big Bang model (for recent reviews see [1–3]).

Even if SBBN is able to reproduce quite well the primordial abundances, still some inconsistency remain: the so called lithium problem. The observation of primordial lithium in metal-poor stars gives an estimate of its abundance relative to the one of Hydrogen of

$$\text{Li}/\text{H}_{\text{exp}} = (1.6 \pm 0.3) \times 10^{-10}, \quad (1.1)$$

where here we reported the experimental value of Ref. [4]. Other experiments performed on different stars and stellar systems give quite consistent results (see among the others [5–7]). On the other hand, the most up-to-date BBN prediction of $^7$Li [8], obtained using the baryon density as measured by the WMAP collaboration [9], is

$$\text{Li}/\text{H}_{\text{th}} = (5.24^{+0.71}_{-0.62}) \times 10^{-10}. \quad (1.2)$$

It is clear, by comparing the two numbers, that there is a discrepancy between the BBN result and the astrophysical observations. This is the so called “first Lithium problem”.

Moreover, in 2006 there was a claim of detection of $^6$Li in old halo stars [10]. In this study, the Authors performed a high resolution observations of Li absorption lines and the abundance of $^6$Li was found to be

$$^6\text{Li}/^7\text{Li} = 5 \times 10^{-2}, \quad (1.3)$$

more than two order of magnitude larger than SBBN predictions. This has been called “second lithium problem”. Further observation and analysis [11–14] showed that three-dimensional modeling of stellar atmosphere which considers non local thermodynamic and includes surface convection can generate asymmetries in the absorption line shape that mimic the presence of $^6$Li. Therefore, the claimed ratio $^6\text{Li}/^7\text{Li}$ is best interpreted as an upper limit, as confirmed by recent data on extremely low metallicity stars [15]. On the other hand, the production of $^6$Li from spallation due to cosmic rays resulted to be the main contribution to cosmological $^6$Li abundance (see e.g. [16]). However, there is not a definite conclusion of this
issue yet and open questions on $^6\text{Li}$ primordial abundance persist.

These discrepancies can have three possible solutions [17]: (1) the presence of systematic errors in the astrophysical observations, (2) the incomplete knowledge of one or more cross-sections of the BBN reaction network or (3) the emergence of new physics beyond SM (BSM). Even if, as in the case of $^6\text{Li}$, the first solution is the most probable, the situation remains still unclear and in particular the last possibility results to be very intriguing. In fact, the existence of BSM relic particles (such as dark matter particles), which can decay or annihilate during the BBN era, can give rise to a series of SM particles which can interact with the BBN network changing light element abundances and potentially solving the lithium problem(s) (see for example Ref. [18] for a review). In this sense, the increasing precision on the input parameters of the SBBN suggests the possibility of using BBN for constraining a wide range of BSM theories (see the reviews of Refs. [2, 3]).

In order to test these exotic scenarios, a great accuracy in the BBN input parameters is needed, in particular in the cross-section of the nuclear reactions involved in the BBN network (or the $S$-factor which is the cross-section net of Coulomb barrier effect). In the last years, a large effort for measuring with high accuracy all the cross-sections of the BBN network in the BBN energy window (50-400 keV) was made by the experimental nuclear community. However, the experimental studies are very difficult, due to the Coulomb barrier which suppresses the cross-sections in the energy window of interest. This translates in larger errors on the experimental data. Therefore, reliable theoretical calculations result fundamental in order to reduce the uncertainties.

In this Thesis we present the theoretical study of two nuclear reactions that are connected to $^6\text{Li}$ abundance in BBN. They are

$$\alpha + d \rightarrow ^6\text{Li} + \gamma, \quad (1.4)$$

and

$$p + ^6\text{Li} \rightarrow ^7\text{Be} + \gamma. \quad (1.5)$$

The study of these reactions is also motivated by the fact that both were object of a recent experimental campaign at the deep underground facility LUNA, at the Gran Sasso National Laboratory [19]. In the following of this Chapter we discuss separately the two reactions, their connection to BBN and the theoretical approaches used for the calculation.

### 1.1 The $\alpha + d \rightarrow ^6\text{Li} + \gamma$ reaction

The $\alpha + d \rightarrow ^6\text{Li} + \gamma$ is considered the main reaction through which $^6\text{Li}$ is produced during BBN [3]. Therefore, it plays a fundamental role in determining $^6\text{Li}$ primordial abundance. Its role is even more important in the case of non-standard BBN, in which there is the possibility of having non-thermal deuteron which can interact with the $^4\text{He}$ environment [17]. For this reason the study of the $S$-factor in the BBN energy window becomes important.

The experimental study of this reaction is very complex not only because of the exponential drop due to the Coulomb barrier, but also because of the isotopic suppression of the multipole $E1$, which is usually the main contributor to the radiative capture reaction cross-sections. For this reason, the experiments, which started in the 1980s with Robertson et al. [20] and then continued in the 1990s [21–24], were able only to give extrapolation or upper limits in the BBN energy window and not
to obtain direct data. Recently, the LUNA Collaboration started a campaign of measurements of this reaction, obtaining for the first time some data points in the BBN window with a direct method [25, 26].

From the theoretical point of view, the study of this reaction, due to the complexity of the problem, has been performed using mainly cluster models [27–31], in which the α particle and the deuteron are considered as structureless particles and their interaction is described by an *ad-hoc* nuclear potential. In such a way the problem reduces to solve a simple two-body equation. Even if these models are able to reproduce the S-factor behavior, the internal structure of the d, α and 6Li nuclei is completely missing. Moreover, in this approach the theoretical uncertainties are not fully controlled and only the Authors of Ref. [31] give an estimate of it by comparing various potential models. In order to recover at least the structure of 6Li, Tursunov et al. [32] constructs the 6Li wave function in a three-body model considering the lithium as an α+p+n system. This permitted to have a more precise description of the final state of the reaction, but still an *ad-hoc* potential is used in order to reproduce the 6Li binding energy. Furthermore, the scattering part is still treated considering the α+d as a two-body problem. It is important to mention that the 6Li can be treated as an *halo* nucleus, in which it is possible to separate the short-range scale of the α particle and the long-range scale of the neutron and proton which form the halo. With this assumption, it is possible to construct a phenomenological cluster interaction by using the so-called halo effective field theory (see for example [33]). The nuclear interactions constructed within this approach are more justifiable from a theoretical point of view and permit also to have reliable estimates of the theoretical errors. However, to our knowledge, there are no published papers which treat the α+d reaction in such approach.

A complete study of the reaction would impose the solution of the six-body problem both for the α+d scattering states and the 6Li bound state and their interaction with photon. Such approach is called an *ab-initio* method. In this approach the nuclear potential models are constructed starting from fundamental theories (i.e. SM) in order to reproduce exactly the interaction among the nucleons. Historically, a series of phenomenological potentials based on the exchange of pions and heavier mesons and then fitted to reproduce the nucleon-nucleon (NN) data sets have been used to study ground states and low-energy scattering states of light nuclei. Examples of these are the Argonne v18 (AV18) [34] or the charge dependent-Bonn2000 (CD-B2k) potentials [35]. These potentials are often used in combination with three-body forces based on the idea that a nucleon can be excited in a Δ particle (for example the Urbana IX (UIX) [36] potential). The use of three-body forces permits to reproduce the experimental energy spectra of the light nuclei. More recently, chiral effective field theory (χEFT) has provided a practical and successful scheme to study two- and many-nucleon interactions [37, 38]. The χEFT approach is based on the observation that the chiral symmetry exhibited by quantum chromodynamics (QCD) has a noticeable impact in the low-energy nuclear dynamics. Therefore, the form of the strong interactions of pions among themselves and with the nucleons is severely constrained by the transformation properties of the fundamental Lagrangian under chiral and discrete symmetries [39–42]. The Lagrangian terms can be organized as an expansion in powers of $Q/\Lambda_\chi$, where $\Lambda_\chi \simeq 1$ GeV specifies the chiral-symmetry-breaking scale and $Q$ is the exchanged pion momentum. This scheme permits to have a control of the theoretical error induced by the truncation of the expansion (see for example [37]). Each Lagrangian term is associated to a low-energy constant (LEC) which is usually determined by fitting two- and three-body experimental data. The nuclear potentials are derived from the
\(\chi\)EFT Lagrangian by using either the time ordering perturbation theory (see for example [43]) or the unitary transformation techniques (see for example [44]). The phenomenological and the chiral nuclear potentials may be then used within the many-body Schrödinger equation to predict other nuclear observables without any new free parameter. Therefore, all the results obtained by using \textit{ab-initio} techniques are independent on the experimental data that one is interested in.

The first attempt to perform an \textit{ab-initio} study of the \(\alpha + d\) radiative capture reaction was performed by Nollett \textit{et al.} [45] by using the Green’s Function Monte Carlo (GFMC) method (see Ref. [46] and references therein) with the AV18/UIX nuclear potential. In that work, the \(^6\text{Li}\) bound state is described as a six-body wave function. However, the \(\alpha + d\) scattering states are still solved in a two-body framework. In a more recent work, Hupin \textit{et al.} [47] have performed for the first time a fully \textit{ab-initio} study of both the bound and the elastic scattering states within the No-Core-Shell-Model (NCSM) framework [48], using a chiral interaction. Those Authors have been able to compute the scattering states by combining the Resonanting Group Model (RGM) with the NCSM [49]. In this approach, the \(A = 6\) bound and scattering wave function have been expanded in terms of the eigenstate of the two-body and four-body Hamiltonian. In such a way, they have been able to obtain a series of coupled channel equations that, solved for positive energies, permitted to obtain the exact asymptotic behavior of the scattering wave functions. With this approach, the Authors have been able to nicely reproduce the \(\alpha + d\) elastic scattering data. However, the calculation of the \(S\)-factor for the \(\alpha + d\) radiative capture is still missing.

In this Thesis we make the first steps towards the calculation of the \(\alpha + d \rightarrow ^6\text{Li} + \gamma\) reaction by using another \textit{ab-initio} approach, the Hyperspherical Harmonic (HH) method. This method was successfully used with \(A \leq 4\) both for scattering and bound states [50] and it is feasible to be extended to larger nuclear systems. In the HH method, the wave function is expanded in HH functions and the quantum mechanical problem is then solved using the the Rayleigh-Ritz variational principle for the bound states and the Kohn variational principle [51] for the scattering states. The idea to use this approach for studying this reaction is very intriguing since, compared to other \textit{ab-initio} method, the HH technique seems to be the best choice for studying low-energy scattering states for nuclear reactions of astrophysical interest [52, 53].

One of the main problems when we consider variational approaches in nuclear physics is the enormous dimension of the basis needed to reach convergence in the expansion of the wave function. In particular, passing from \(A = 4\) to \(A = 6\), the dimension of the basis grows exponentially, making hard the practical use of the HH expansion. Therefore, one aim of this Thesis is to introduce some technical improvements on the numerical implementation allowing for the extension of the HH approach. After that, we will focus on the calculation of the ground state of \(^6\text{Li}\) which is the final state of the reaction. The importance of this nucleus goes beyond its relevance in the BBN. In fact, it is the first stable nucleus beyond the \(A = 5\) mass gap and it is weakly bound. Therefore, it is a good laboratory for studying nuclear force, since its exotic structure must emerge directly from the nuclear force itself. An important intermediate goal of this Thesis will be the study of the Asymptotic Normalization Coefficient (ANC). The ANC is the normalization of the tail of the \(^6\text{Li}\) wave function when projected on the \(\alpha + d\) cluster, and it can be extracted experimentally. Since in the BBN energy window the nuclear reactions are almost peripheral, only the tail of the wave functions is involved and so the \(S\)-factor is proportional to the square of the ANC. It is clear then that the knowledge of the
ANC is a fundamental ingredient to determine the $S$-factor. The calculation of this observable is very complex since we need to construct in the same ab-initio framework the $\alpha$ and the $d$ wave function combining it with the $^6\text{Li}$ one. Moreover, the computation of the ANC has, from the technical point of view, a lot in common with the calculation of the scattering states. Therefore, it can be considered the first step towards the construction of the HH wave function of the $\alpha + d$ scattering states.

### 1.2 The $p + ^6\text{Li} \rightarrow ^7\text{Be} + \gamma$ reaction

The $p + ^6\text{Li} \rightarrow ^7\text{Be} + \gamma$ reaction is not considered to play a direct role in the BBN since the small amount of $^6\text{Li}$ present in the early Universe environment. However, its cross-section is directly connected to the $^7\text{Be} + \gamma \rightarrow p + ^6\text{Li}$ reaction, through the detailed balance principle. The latter reaction is supposed to become an important contributor to $^6\text{Li}$ abundance in case of presence of high energy non-thermal photons generated by the decay of BSM particles during the BBN [54].

The $p + ^6\text{Li} \rightarrow ^7\text{Be} + \gamma$ cross-section was extensively studied in the past by many experimental groups [55–59]. However, large uncertainties in the $S$-factor at the BBN energies remain. Furthermore, a recent work [59] has pointed out the possible presence of a resonance in the BBN energy window, with subsequent suppression at zero energy. In order to confirm or reject such possibility, the LUNA Collaboration has also performed a new campaign of measurements in the Spring of 2018.

The extrapolation of the astrophysical $S$-factor at zero-energy has been performed within the R-matrix approach in Ref. [60], including somewhat by hand the resonance-like structure proposed in Ref. [59]. On the other hand, all theoretical calculations performed within the cluster model framework do not reproduce the claimed resonance. The most important theoretical studies were performed using different approaches, like a two-body phenomenological potential [61, 62], an optical potential [63], a four-cluster model [64] and the Gamow shell model [65], obtaining all quite consistent results with each other. However, all these studies are lacking of an estimate of the theoretical uncertainty, especially that arising from model dependence.

In this Thesis, we present a new theoretical study within a cluster model of the $p + ^6\text{Li} \rightarrow ^7\text{Be} + \gamma$, using also a two-body phenomenological potential similar to that of Ref. [62], but calculating not only the astrophysical $S$-factor, but also the angular distribution of the emitted photon, for which there are also available data [56]. The main goal of this work is to give to the LUNA Collaboration, which is finalizing the data analysis on this reaction, a reliable theoretical calculation of the angular distribution which enters in the determination of the efficiency of the detector. Moreover, we also estimate a “theoretical” error bar, based on the different cluster approaches presented in literature. Finally, we investigate on the possible presence of the resonance structure as suggested by the data of Ref. [59].

This thesis is divided in two parts. In the first part we discuss the first steps towards the ab-initio calculation of the $\alpha + d$ radiative capture. In particular in Chapter 2 we present the HH formalism for $A = 6$ focusing on the solution of the bound state problem. In Chapter 3 we discuss the results obtained for the $^6\text{Li}$ ground state. Moreover, in this Chapter we analyze also the electromagnetic properties of $^6\text{Li}$, namely its charge radius, its magnetic dipole and its electric quadrupole. Finally, in Chapter 4 we study the $\alpha + d$ clusterization of $^6\text{Li}$ in order to determine the ANC. The second part of the Thesis is instead dedicated to the phenomenological
study of the $p + ^{6}\text{Li} \rightarrow ^{7}\text{Be} + \gamma$ reaction. This study, published in Ref. [66], is presented in Chapter 5 of this Thesis. Lastly, we conclude in Chapter 6 by discussing possible future development and applications of this work. A series of technical details on the calculation and the implementation of the HH method are given in the Appendices.
Chapter 2

The Hyperspherical Harmonic method for bound states

In this chapter we present the formalism needed to solve the Schrödinger equation for the bound state of $^6$Li by using the HH functions. The HH method is a variational approach in which the wave function is expanded in terms of basis states constructed with the HH functions, transforming the problem of solving the Schrödinger equation in an eigenvalue problem. This chapter is organized as follows. We start by defining the Jacobi vectors and the hyperspherical variables in Section 2.1 and by constructing the HH functions in Section 2.2. Then in Section 2.3 we will define the basis states by including the spin and isospin quantum numbers. In Section 2.4 we present the eigenvalue problem and we discuss the construction of the Hamiltonian matrix elements. The last section is dedicated to some technical details on the calculation of the potential matrix elements.

In this Thesis we will consider also the wave function of $^4$He. The construction of the $^4$He wave function follows the same procedure described in this chapter. However, specific details can be found in Ref. [50].

2.1 Jacobi coordinates and Hyperspherical variables

A nucleus can be considered as a generic isolated system of $A$ particles with spatial coordinates $\mathbf{r}_i$ and masses $m_i$, $i = 1, \ldots, A$. We want to study the system in the center-of-mass (c.m.) frame, by decoupling the c.m. motion in the Schrödinger equation. What remains are $N = A - 1$ vectors which describe the internal spatial configurations. In order to do that, we introduce the Jacobi vectors $\mathbf{x}_i$, $i = 1, \ldots, N$, which, by definition, are such that the total kinetic energy operator can be written as

$$
T = -\sum_{i=1}^{A} \frac{\hbar^2}{2m_i} \nabla_i^2 = \frac{\hbar^2}{m} \sum_{i=1}^{N} \nabla^2_{\mathbf{x}_i} - \frac{\hbar^2}{2M} \nabla^2_X ,
$$

(2.1)

where $m$ is a reference mass, $M = \sum_{i=1}^{A} m_i$ is the total mass of the system, and $X = (1/M) \sum_{i=1}^{A} m_i \mathbf{r}_i$ is the c.m. coordinate. In this Thesis we consider all the particles to have equal mass $m = m_p$, being $m_p \simeq m_n$, where $m_p$ is the proton mass and $m_n$ the neutron mass. There are various possible choices of the Jacobi vectors. In particular we refer as “standard” set of Jacobi vectors to the following choice

$$
\mathbf{x}_{N-j+1} = \sqrt{\frac{2j}{j+1}} [\mathbf{r}_{j+1} - X_j] , \quad j = 1, \ldots, N ,
$$

(2.2)
Chapter 2. The Hyperspherical Harmonic method for bound states

with

\[ X_j = \frac{1}{j} \sum_{i=1}^{j} r_i \]  

(2.3)

Explicitly, for \( A = 6 \) this choice gives

\[ x_{1p} = \sqrt{\frac{5}{3}} \left( r_n - \frac{r_m + r_l + r_k + r_j + r_i}{5} \right) \]
\[ x_{2p} = \sqrt{\frac{8}{5}} \left( r_m - \frac{r_l + r_k + r_j + r_i}{4} \right) \]
\[ x_{3p} = \sqrt{\frac{3}{2}} \left( r_l - \frac{r_k + r_j + r_i}{3} \right) \]
\[ x_{4p} = \sqrt{\frac{4}{3}} \left( r_k - \frac{r_j + r_i}{2} \right) \]
\[ x_{5p} = r_j - r_i , \]  

(2.4)

where \((i, j, k, l, m, n)\) indicates a generic permutation \(p\) of the particles. By definition the reference permutation \(p = 1\) is chosen to correspond to the order \((1, 2, 3, 4, 5, 6)\) of the particles. There exists other possible choices for the Jacobi vectors. For example when we want to describe the \(4 + 2\) cluster structure of \(^6\)Li, namely \(\alpha + d\), a more suitable choice of the Jacobi coordinates is

\[ x_{1Bp} = r_n - r_m \]
\[ x_{2Bp} = \sqrt{\frac{8}{3}} \left( r_n + r_m - \frac{r_l + r_k + r_j + r_i}{4} \right) \]
\[ x_{3Bp} = \sqrt{\frac{3}{2}} \left( r_l - \frac{r_k + r_j + r_i}{3} \right) \]
\[ x_{4Bp} = \sqrt{\frac{4}{3}} \left( r_k - \frac{r_j + r_i}{2} \right) \]
\[ x_{5Bp} = r_j - r_i , \]  

(2.5)

which we name set \(B\). The basis elements can be defined using any definition of the Jacobi coordinates. The completeness of the basis ensures that the expansions are completely equivalent using any set of Jacobi vectors. In numerical applications the expansion is truncated and this equivalence does not hold anymore. In this Thesis we will use the “standard” set for the expansion of the ground state of \(^6\)Li, while we will consider the set \(B\) when we will study \(\alpha + d\) states.

For a given choice of the Jacobi vectors, the hyperspherical coordinates are given by the hyperradius \(\rho\), which is independent on the permutation order of the particles and is defined as

\[ \rho = \sqrt{\sum_{i=1}^{N} x_{ip}^2} = \sqrt{\frac{2}{N} \sum_{i=1}^{N} (r_i - X)^2} , \]  

(2.6)

and by a set \(\Omega_{Np}\) of angular variables. For the bound state calculation, we use the Zernike and Brinkman representation [67,68], where there are \(2N\) polar angles \(\hat{x}_{ip} = (\theta_{ip}, \phi_{ip})\) of the Jacobi vectors \(x_{ip}\), \(i = 1, \ldots, N\), and \(N - 1\) hyperspherical
angles $\varphi_{ip}$, with $0 \leq \varphi_{ip} \leq \pi/2$, given by
\[
\cos \varphi_{ip} = \frac{x_{ip}}{\sqrt{x_{1p}^2 + \cdots + x_{ip}^2}}, \quad i = 2, \ldots, N, \tag{2.7}
\]
where $x_{ip}$ is the modulus of the Jacobi vector $x_{ip}$. Therefore we have
\[
\Omega_{Np} = \{\hat{x}_{1p}, \cdots, \hat{x}_{Np}, \varphi_{2p}, \cdots, \varphi_{Np}\}. \tag{2.8}
\]
As for the Jacobi coordinates, there are other possible definitions for the hyperspherical angles $\varphi_{ip}$. We explicitly discuss them and their utility in the next Chapters.

### 2.2 Hyperspherical Harmonic Functions

The spherical harmonic functions $Y_{\ell,m}(\theta, \phi)$ are very widely used in the study of quantum mechanical problem in a three-dimensional space. In this section we construct the generalization of the spherical harmonics to the $D = 3N$ dimensional space, namely the HH functions. For simplicity we use only the “standard” definitions of the Jacobi vectors and of the hyperspherical coordinates [Eqs. (2.4) and (2.7)], however all the results can be generalized to any set of Jacobi vector and hyperspherical coordinates. Moreover, the results are independent of the permutation of the particles, therefore we discard $p$ in the notation.

The $3N$-dimensional Laplace operator $\Delta$, which appears in the kinetic energy, can be written as
\[
\Delta = \sum_{i=1}^{N} \nabla_{x_i}^2 = \left( \frac{\partial^2}{\partial \rho^2} + \frac{3N - 1}{\rho} \frac{\partial}{\partial \rho} + \frac{\Lambda_{N}^2(\Omega_N)}{\rho^2} \right), \tag{2.9}
\]
where $\Lambda_{N}^2$ is the $3N$-dimensional generalized angular momentum operator depending only on the hyperangles $\Omega_N$. An homogeneous polynomial $p_{[K]}$ of degree $K$ in the Cartesian coordinates of $N$ Jacobi vectors, gives $\Delta p_{[K]} = 0$. We can rewrite it in the form
\[
p_{[K]} = \rho^K Y_{[K]}, \tag{2.10}
\]
where $\rho$ is the hyperradius as given in Eq. (2.6) and $Y_{[K]}$ depends only on the variables $\Omega_N$ defined in Eq. (2.8), being $p_{[K]}$ an homogeneous polynomial. Applying $\Delta$ to Eq. (2.10) we get
\[
\Delta p_{[K]} = \left( \frac{\partial^2}{\partial \rho^2} + \frac{3N - 1}{\rho} \frac{\partial}{\partial \rho} + \frac{\Lambda_{N}^2(\Omega_N)}{\rho^2} \right) \rho^K Y_{[K]}(\Omega_N) = 0
\]
\[
= \left( \Lambda_{N}^2(\Omega_N) + K(K + D - 2) \right) \rho^{K-2} Y_{[K]}(\Omega_N) = 0, \tag{2.11}
\]
and dividing by $\rho^{K-2}$ we get
\[
\left( \Lambda_{N}^2(\Omega_N) + K(K + D - 2) \right) Y_{[K]}(\Omega_N) = 0. \tag{2.12}
\]

The functions that satisfies the latter equation are known as Hyperspherical Harmonic functions. This is the eigenfunction of the generalized angular momentum operator $\Lambda_{N}^2$ which is sometimes called the grand angular momentum operator. $K$
is called the grand angular quantum number while \([K]\) represents a set of quantum numbers as specified in the following.

The grand angular momentum operator can be written in the form [68]

\[
\Lambda_i^2(\Omega_i) = \frac{\partial^2}{\partial \varphi_i^2} + \left[ 3(i - 2)\cot \varphi_i + 2(\cot \varphi_i - \tan \varphi_i) \right] \frac{\partial}{\partial \varphi_i} + \frac{L_i^2}{\cos^2 \varphi_i} + \frac{\Lambda_i^2(\Omega_{i-1})}{\sin^2 \varphi_i},
\]

where \(L_i^2\) is the angular momentum operator associated with the \(i\)-th Jacobi vector. In particular

\[
\Lambda_1^2(\Omega_1) = L_1^2.
\]

The solutions of Eq. (2.12) can be constructed by following a recursive procedure [67]. In particular

\[
\Lambda_{i+1}^2(\Omega_{i+1}) = \frac{\partial^2}{\partial \varphi_{i+1}^2} + \left[ 3(i + 1)\cot \varphi_{i+1} + 2(\cot \varphi_{i+1} - \tan \varphi_{i+1}) \right] \frac{\partial}{\partial \varphi_{i+1}} + \frac{L_{i+1}^2}{\cos^2 \varphi_{i+1}} + \frac{\Lambda_{i+1}^2(\Omega_i)}{\sin^2 \varphi_{i+1}},
\]

where \(\Lambda_{i+1}^2(\Omega_{i+1})\) is a function to be determined. Defining \(\rho = \cos \varphi_{i+1}\), Eq. (2.15) reduces to the form

\[
\Lambda_2(\Omega_2)Y_{[K]}(\Omega_2) = -K(K + 4)Y_{[K]}(\Omega_2), \quad \Omega_2 \equiv \{\hat{x}_1, \hat{x}_2, \varphi_2\}.
\]

Let us look for a solution of the previous equation of the form

\[
Y_{[K]}(\Omega_2) = F(\cos 2\varphi_2)(\cos \varphi_2)\ell_2(\sin \varphi_2)\ell_1 Y_{\ell_1m_1}(\hat{x}_1)Y_{\ell_2m_2}(\hat{x}_2),
\]

where \(F\) is a function to be determined. Defining \(y = \cos 2\varphi_2\), Eq. (2.15) reduces to

\[
(1 - y^2)F'' + (\alpha - \beta y)F' + \gamma F = 0,
\]

where

\[
\alpha = \ell_2 - \ell_1, \quad \beta = \ell_1 + \ell_2 + 3, \quad \gamma = \frac{1}{4} [K(K + 4) - (\ell_1 + \ell_2)(\ell_1 + \ell_2 + 4)].
\]

Eq. (2.17) is the one satisfied by the Jacobi polynomial \(P_n^{\ell_1+1/2,\ell_2+1/2}(z)\) provided that \(K = 2n + \ell_1 + \ell_2\) [69]. Therefore, a solution of Eq. (2.15) is given by

\[
Y_{[K]}(\Omega_2) = N_n^{\ell_2,\nu_2}(\cos \varphi_2)\ell_2(\sin \varphi_2)\ell_1 Y_{\ell_1m_1}(\hat{x}_1)Y_{\ell_2m_2}(\hat{x}_2) P_n^{\ell_1+1/2,\ell_2+1/2}(\cos 2\varphi_2),
\]

where \(N_n^{\ell_2,\nu_2}\) is a normalization factor which will be specified later and \(\nu_2 = 2n + \ell_1 + \ell_2 + 2\). For \(N = 2\) the symbol \([K]\) results to be

\[
[K] = \{\ell_1, m_1, \ell_2, m_2, n\}.
\]

We can now verify that \(\rho^KY_{[K]}(\Omega_2)\) is an homogeneous polynomial of degree \(K\) in the Cartesian component \(x_1\) and \(x_2\). Using the fact that \(x_1 = \rho \sin \varphi_2\) and \(x_2 = \rho \cos \varphi_2\), we can write

\[
\rho^KY_{[K]}(\Omega_2) = N_n^{\ell_2,\nu_2} \rho^{2n} x_1^{\ell_1} Y_{\ell_1m_1}(\hat{x}_1) x_2^{\ell_2} Y_{\ell_2m_2}(\hat{x}_2) P_n^{\ell_1+1/2,\ell_2+1/2}(\cos 2\varphi_2).
\]
The terms $x_1^{\ell_1}Y_{\ell_1 m_1}(\hat{x}_1)$ and $x_2^{\ell_2}Y_{\ell_2 m_2}(\hat{x}_2)$, are homogeneous polynomials of degree $\ell_1$ and $\ell_2$. We remain with

$$\rho^{2n}P_n^{\ell_1+1/2,\ell_2+1/2}(\cos 2\varphi_2) = \rho^{2n} \sum_{m=0}^{n} a_m (\cos 2\varphi_2)^m$$

$$= \sum_{m=0}^{n} a_m (\rho^2 \cos 2\varphi_2)^m \rho^{2(n-m)} = \sum_{m=0}^{n} a_m (x_2^2 - x_1^2)(x_2^2 + x_1^2)^{n-m},$$

(2.22)

which is an homogeneous polynomial of degree $2n$. In Eq. (2.22) we have used $\rho^2 \cos 2\varphi_2 = x_2^2 - x_1^2$ and the definition of Jacobi polynomials [69]. In conclusion $\rho^K Y_{[K]}(\Omega_2)$ is a homogeneous polynomial of degree $K = 2n + \ell_1 + \ell_2$.

We can now construct the HH functions for any $N$. Let us suppose we know the solution in the case $N - 1$, namely the function $Y_{[K_{N-1}]}(\Omega_{N-1})$, which satisfies the equation

$$\Lambda_{N-1}^2(\Omega_{N-1})Y_{[K_{N-1}]}(\Omega_{N-1}) = -K_{N-1}(K_{N-1} + D - 5)Y_{[K_{N-1}]}(\Omega_{N-1}),$$

(2.23)

where $K_{N-1}$ is the corresponding grand angular quantum number. Analogously to Eq. (2.16), we can look for the expression of the HH function can therefore be cast in the form [68]

$$\Lambda_N^2(\Omega_N)Y_{[K]}(\Omega_N) = (\cos \varphi_N)^{\ell_N}(\sin \varphi_N)^{K_{N-1}}Y_{[K_{N-1}]}(\Omega_{N-1})Y_{\ell_N m_N}(\hat{x}_N)F(\cos 2\varphi_N).$$

(2.24)

By inserting this expression for $Y_{[K]}$ in the corresponding eigenvalue equation and taking into account Eq. (2.23), we get the following solution

$$F(\cos 2\varphi_N) = N_{\ell_N, \nu_N}^{\ell_N, \nu_N} P_n^{\ell_N+1/2}(\cos 2\varphi_N),$$

(2.25)

with

$$K = 2n_N + \ell_N + K_{N-1}, \quad \nu_{N-1} = K_{N-1} + \frac{3(N-1)}{2} - 1,$$

(2.26)

$$\nu_N = K + \frac{3N}{2} - 1.$$
normalization factors $N$ are chosen to verify the orthonormal condition
\[
\int d\Omega_N \left(Y_{[K]}(\Omega_N)\right)^* Y_{[K']} (\Omega_N) = \delta_{[K],[K']},
\] (2.30)
where $N$
\[
d\Omega_N = \sin \theta_1 d\theta_1 d\phi_1 \prod_{j=2}^{N} \sin \theta_j d\theta_j d\phi_j (\cos \varphi_j)^2 (\sin \varphi_j)^{3j-4} d\varphi_j
\] (2.31)
is the surface element on the hypersphere of unit hyperradius. To be noticed that the integral over all the Jacobi coordinates can be rewritten in terms of $d\Omega_N$ and the hyperradius, namely
\[
\int \prod_{i=1}^{N} d^3x_i = \int dp^{3N-1} \int d\Omega_N .
\] (2.32)
The explicit expression for $N$ is
\[
N_{\ell_j}^{\nu_j,n_j} = \left[ \frac{2\nu_j \Gamma(\nu_j - n_j)n_j!}{\Gamma(\nu_j - n_j - \ell_j - \frac{1}{2})\Gamma(n_j + \ell_j + \frac{3}{2})} \right]^{1/2}.
\] (2.33)
We need now to verify that $\rho^K Y_{[K]}$ is a homogeneous polynomial in the Cartesian Jacobi coordinates. It is easy, using Eq. (2.7), to verify that
\[
\rho^K Y_{[K]}(\Omega_N) \propto \prod_{j=1}^{N} x_j^{\ell_j} Y_{\ell_j,m_j}(\hat{x}_j)
\] (2.34)
\[
\times \prod_{j=2}^{N} \rho^{2n_j} (\sin \varphi_j + \cdots + \sin \varphi_N)^{2n_j} P_{n_j}^{\nu_j-1,\ell_j} (\cos 2\varphi_j).
\] (2.35)
The first term, in Eq. (2.34) is a homogeneous polynomial of degree $\ell_1 + \cdots + \ell_N$. The second term can be rewritten as
\[
(\rho \sin \varphi_j + \cdots + \sin \varphi_N)^{2n_j} P_{n_j}^{\nu_j-1,\ell_j} (\cos 2\varphi_j)
\] (2.36)
\[
= \rho^{2n_j} (\sin \varphi_j + \cdots + \sin \varphi_N)^{2n_j} \sum_{m=0}^{n_j} a_m (\cos 2\varphi_j)^m
\] (2.37)
where we used the following relations
\[
\rho^2 \cos 2\varphi_j = \frac{x_j^2 - (x_1^2 + \cdots + x_{j-1}^2)}{(\sin \varphi_j + \cdots + \sin \varphi_N)^2},
\] (2.38)
and
\[
(\rho \sin \varphi_j + \cdots + \sin \varphi_N)^2 = x_1^2 + \cdots + x_j^2.
\] (2.39)
Using Eq. (2.35), the second term in Eq. (2.34) results to be a homogeneous polynomial of order $2 \sum_{j=2,N} n_j$. Therefore, the function $\rho^K Y_{[K]}$ is an homogeneous polynomial of order $K = \ell_1 + \sum_{j=2,N} (\ell_j + 2n_j)$ in the Jacobi coordinates.
The HH functions have several important properties. Here we report only the completeness of the HH basis without proof. By introducing the hypercoordinates \( \rho', \Omega'_N \) associated with the \( N \) vectors \( x_i' \), it is possible to show that [50]

\[
\sum_{[K]} Y^*_{[K]}(\Omega'_N)Y_{[K]}(\Omega_N) = \delta^{D-1}(\Omega_N - \Omega'_N) ,
\]

where

\[
\delta^{D-1}(\Omega_N - \Omega'_N) = \frac{1}{\prod_{i=1}^{N} \delta^{2}(\hat{x}_i - \hat{x}'_i) \prod_{i=2}^{N} \delta(\varphi_i - \varphi'_i)} .
\]

As a consequence, every continuous function \( f(\Omega_N) \) can be expanded in terms of the HH functions as

\[
f(\Omega_N) = \int d\Omega'_N \delta^{D-1}(\Omega_N - \Omega'_N) f(\Omega'_N) = \sum_{[K]} a_{[K]} Y_{[K]}(\Omega_N) ,
\]

where

\[
a_{[K]} = \int d\Omega'_N Y^*_{[K]}(\Omega'_N) f(\Omega'_N) .
\]

We will use this property very widely in the following of this Thesis.

In this work we will use HH functions with definite total angular momentum \( L \). They are constructed using the following coupling scheme [50]

\[
\mathcal{Y}_{\mu}^{KLM}(\Omega_N) = \sum_{m_1, \ldots, m_N} (\ell_1 m_1 \ell_2 m_2 | L_2 M_2)(L_2 M_2 \ell_3 m_3 | L_3 M_3) \times \cdots \times (L_{N-1} M_{N-1} \ell_N m_N | LM) Y_{[K]}(\Omega_N) ,
\]

where \( Y_{[K]}(\Omega_N) \) is defined in Eq. (2.27), \( (\ell_1 m_1 \ell_2 m_2 | L_2 M_2) \) and so on are Clebsch-Gordan coefficients and \( M_i = \sum_{j=1,4} m_j \). The symbol \( \mu \) represent the complete set of quantum number, namely

\[
\mu \equiv \{ \ell_1, \ldots, \ell_N, L_2, \ldots, L_{N-1}, n_2, \ldots, n_N \} .
\]

Reintroducing the notation for the permutations, the final expression of the HH function for the case \( A = 6 \) is

\[
\mathcal{Y}_{\mu}^{KLM}(\Omega_{5p}) = \left( \left( (Y_{\ell_1}(\hat{x}_{1p})Y_{\ell_2}(\hat{x}_{2p})Y_{\ell_3}(\hat{x}_{3p}) \right)_{L_2} Y_{\ell_4}(\hat{x}_{4p}) \right)_{L_3} Y_{\ell_5}(\hat{x}_{5p}) \right)_{LM} \times \mathcal{P}_{n_2,n_3,n_4,n_5}(\varphi_{2p}, \varphi_{3p}, \varphi_{4p}, \varphi_{5p}) ,
\]

where

\[
\mathcal{P}_{n_2,n_3,n_4,n_5}(\varphi_{2p}, \varphi_{3p}, \varphi_{4p}, \varphi_{5p}) = N_{n_2}^{\ell_2,\mu_2}(\cos \varphi_{2p})^{\ell_2}(\sin \varphi_{2p})^{\ell_1} P_{n_2}^{\ell_1+1/2,\ell_2+1/2}(\cos 2\varphi_{2p}) \times N_{n_3}^{\ell_3,\mu_3}(\cos \varphi_{3p})^{\ell_3}(\sin \varphi_{3p})^{\ell_2} P_{n_3}^{\ell_2+1/2,\ell_3+1/2}(\cos 2\varphi_{3p})
\]

\[
\times N_{n_4}^{\ell_4,\mu_4}(\cos \varphi_{4p})^{\ell_4}(\sin \varphi_{4p})^{\ell_3} P_{n_4}^{\ell_3+1/2,\ell_4+1/2}(\cos 2\varphi_{4p})
\]

\[
\times N_{n_5}^{\ell_5,\mu_5}(\cos \varphi_{5p})^{\ell_5}(\sin \varphi_{5p})^{\ell_4} P_{n_5}^{\ell_4+1/2,\ell_5+1/2}(\cos 2\varphi_{5p}) ,
\]

and

\[
\mu \equiv \{ \ell_1, \ell_2, \ell_3, \ell_4, \ell_5, L_2, L_3, L_4, n_2, n_3, n_4, n_5 \} .
\]
2.3 The Hyperspherical Harmonic expansion

In the following we will use the isospin formalism. Therefore, each nucleon will be described by its position and spin-isospin projection. Since the nucleons are Fermions, the wave function of the six-nucleon system has to be antisymmetric under the exchange of any pair of particles. Moreover, we require that our wave function has a well defined total angular momentum \( J, J_z \) and parity \( \pi \). Therefore, we define a complete basis of antisymmetrical hyperangular-spin-isospin states as follows

\[
\Psi_{KLSTJ\pi}^{\alpha} = \sum_{p=1}^{N_p} \phi_{KLSTJ\pi}^{\alpha}(i, j, k, l, m, n),
\]

where with \( p \) we indicate a generic even permutation of the six particles, \( p \equiv (i, j, k, l, m, n) \), \( N_p \) being the total number of even permutation given by

\[
N_p = \frac{6!}{2} = 360,
\]

and

\[
\phi_{KLSTJ\pi}^{\alpha}(i, j, k, l, m, n) = \begin{aligned}
\gamma^{KLM}_{\mu} (\Omega_{5p}) & \left[ \left( (s_is_j)_{S_2} s_k \right)_{S_3} \left( (s_is_m)_{S_4} s_n \right)_{S_5} \right]_S \bigg\} \bigg\}\bigg\}
& \otimes \left[ \left( (t_it_j)_{T_2} t_k \right)_{T_3} \left( (t_it_m)_{T_4} t_n \right)_{T_5} \right]_{T, T_z}.
\end{aligned}
\]

The function \( \gamma^{KLM}_{\mu} (\Omega_{5p}) \) is the HH function defined in Eq. (2.44) and \( s_i \) (\( t_i \)) denotes the spin (isospin) function of nucleon \( i \). To be noticed that the coupling scheme of the spin (isospin) does not follow the one of the hyperangular part. This particular choice simplifies the calculations of the potential matrix elements. There are other possible choices for the coupling of the spin (isospin) states that can be easily connected through combinations of 6j- and 9j-Wigner coefficients. The total orbital angular momentum \( L \) of the HH function is coupled to the total spin \( S \) to give the total angular momentum \( J, J_z \). while the total isospin is given by \( T, T_z \). The index \( \alpha \) labels the possible choice of hyperangular, spin and isospin quantum numbers,

\[
\alpha \equiv \{ \ell_1, \ell_2, \ell_3, \ell_4, \ell_5, \ell_6, \ell_7, \ell_8, \ell_9, \ell_10, \ell_11, \ell_12 \},
\]

compatible with the given values of \( K, L, S, T, J, \) and \( \pi \). The parity of the state is \( \pi = (-1)^{\ell_1+\ell_2+\ell_3+\ell_4+\ell_5} \) and we will include in our basis only the states such that \( \pi \) corresponds to the parity of the nuclear state under study.

The total wave function must be completely antisymmetric under the exchange of any pair of particles. Therefore we need to impose antisymmetry on each state \( \Psi_{KLSTJ\pi}^{\alpha} \). For example, after the permutation of any pair, the state given in Eq. (2.47) can be rearranged so that

\[
\Psi_{KLSTJ\pi}^{\alpha} \rightarrow \sum_{p=1}^{360} \phi_{KLSTJ\pi}^{\alpha}(j, i, k, l, m, n).
\]
Chapter 2. The Hyperspherical Harmonic method for bound states

15

Therefore to have antisymmetry it is sufficient to have

\[ \Phi_{KLST J\pi}^{\alpha}(j,i,k,l,m,n) = -\Phi_{KLST J\pi}^{\alpha}(i,j,k,l,m,n). \] (2.52)

Under the exchange of \( i \leftrightarrow j \) the Jacobi vector \( x_{5p} \) [Eq. (2.4)] changes its sign, whereas all the others remain the same. Therefore, the HH function \( Y_{KLST J\pi}^{\alpha}(\Omega_{5p}) \) in Eq. (2.44) transforms into itself times a factor \((-1)^{\ell_5}\). The spin-isospin part [see Eq. (2.49)] part transforms into itself times a factor \((-1)^{S_2+T_2}\) for the \( i \leftrightarrow j \) exchange. Therefore, we obtain

\[ \Phi_{KLST J\pi}^{\alpha}(j,i,k,l,m,n) = (-)^{\ell_5+S_2+T_2} \Phi_{KLST J\pi}^{\alpha}(i,j,k,l,m,n), \] (2.53)

In order to fulfill the condition of Eq. (2.52) we impose the condition

\[ \ell_5 + S_2 + T_2 = \text{odd}, \] (2.54)

on the quantum numbers of the HH states. In such a way we construct only antisymmetric states.

2.3.1 Orthogonalization of the basis

The number \( M_{KLST J\pi} \) of antisymmetric functions \( \Psi_{KLST J\pi}^{\alpha} \) with fixed \( K, L, S, T, J \) and \( \pi \) in general is very large, due to the high number of possible combinations of quantum numbers \( \alpha \) that fulfill the requirement of antisymmetry and parity. However, the sum over the permutations in Eq. (2.47) generates states that are linearly dependent among each other. This means that our basis is overcomplete and we need to extract only the independent states. In order to do that we use the Transformation Coefficients (TC) \( a_{KLST J\pi}^{\alpha,\alpha'}(p) \) defined as

\[ \Phi_{KLST J\pi}^{\alpha}(i,j,k,l,m,n) = \sum_{\alpha'} a_{KLST J\pi}^{\alpha,\alpha'}(p) \Phi_{KLST J\pi}^{\alpha'}(1,2,3,4,5,6). \] (2.55)

Hence, the states \( \Psi_{KLST J\pi}^{\alpha} \) of Eq. (2.47) can be written as

\[ \Psi_{KLST J\pi}^{\alpha} = \sum_{\alpha'} A_{KLST J\pi}^{\alpha,\alpha'} \Phi_{KLST J\pi}^{\alpha'}(1,2,3,4,5,6), \] (2.56)

where

\[ A_{KLST J\pi}^{\alpha,\alpha'} = \sum_{p=1}^{360} a_{KLST J\pi}^{\alpha,\alpha'}(p). \] (2.57)

The coefficients \( A_{KLST J\pi}^{\alpha,\alpha'} \) contain all the properties of our basis, and so the knowledge of all of them coincides with the knowledge of the entire basis. Moreover, they permit to simplify the determination of the independent states as well as the calculation of the matrix elements, as we will see in the next section. We will discuss the explicit calculation of the TC \( a_{KLST J\pi}^{\alpha,\alpha'}(p) \) and some of their properties in Appendix A. For now we suppose we are able to compute them.

The fundamental ingredient to identify the independent states is the knowledge of the norm matrix elements

\[ N_{KLST J\pi}^{\alpha,\alpha'} = \langle \Psi_{KLST J\pi}^{\alpha} | \Psi_{KLST J\pi}^{\alpha'} \rangle_{\Omega}, \] (2.58)
where \( \langle \cdots | \cdots \rangle_\Omega \) denotes the spin and isospin trace and the integration over the hyperspherical variables. Using the orthogonality of the HH basis with Eq. (2.56) we obtain

\[
N_{\alpha,\alpha'}^{KLST J\pi} = \sum_{\alpha''} (A_{\alpha,\alpha''}^{KLST J\pi})^* A_{\alpha',\alpha''}^{KLST J\pi},
\]

(2.59)

and also

\[
\langle \Psi_{\alpha}^{KLST J\pi} | \Psi_{\alpha'}^{K'L'S'T'J'\pi'} \rangle_\Omega = 0 \quad \text{for} \quad \{KLST J\pi\} \neq \{K'L'S'T'J'\pi'\}.
\]

(2.60)

Once the matrix elements \( N_{\alpha,\alpha'}^{KLST J\pi} \) are evaluated, the orthogonalization procedure presented in Appendix A.3 is used to find and eliminate the linearly dependent states among the various \( \Psi_{\alpha}^{KLST J\pi} \) functions.

The number of independent antisymmetric states \( M_{KLST J\pi}' \) is noticeably smaller than the corresponding \( M_{KLST J\pi} \) as can be seen in Table 2.1, where we report the values of \( M_{KLST J\pi} \) and \( M_{KLST J\pi}' \) for the case \( J = 1, T = 0 \) and \( \pi = + \), which corresponds to the ground state of the \( ^6\text{Li} \) up to \( K = 10 \). Observing the table it is possible to notice that the number of states starts to be very large already for \( K = 6 \). For the case \( K = 0 \) and \( LST J\pi = 0101^+ \), there is no independent state due to the Pauli principle. The number of states with \( S = 3 \) is very small compared to the others, because the spin states which can be constructed are only symmetric. In Figure 2.1 we plotted both \( M_{0101^+} \) and \( M_{0101^+}' \) as function of \( K \). As can be seen from the figure, the number of independent states is \( \sim 2 \) orders of magnitude less than the total number of antisymmetric states. It is also interesting to notice that the ratio \( M_{0101^+}/M_{0101^+}' \) is almost constant varying \( K \). Moreover, from the figure it is clear the exponential growing of \( M_{0101^+} \) and \( M_{0101^+}' \) as function of \( K \). A similar behavior was found for all the combinations \( LST \) considered in Table 2.1.

![Figure 2.1: Number of states for the case \( LST J\pi = 0101^+ \) as function of the grandangular quantum number \( K \). The red circles are the total number of antisymmetric states \( M_{KLST J\pi} \) while the blue triangles are the number of linearly independent antisymmetric states \( M_{KLST J\pi}' \). To be noticed that the y-axis is in logarithmic scale. The lines are added to guide the eyes.](image-url)
| $K$ | $L = 0$ | $S = 1$ | $L = 2$ | $S = 1$ | $L = 2$ | $S = 2$ | $L = 2$ | $S = 3$ | $L = 1$ | $S = 0$ | $L = 1$ | $S = 1$ | $L = 1$ | $S = 2$ |
|-----|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
|     | $M_{K0101+}$ | $M'_{K0101+}$ | $M_{K2101+}$ | $M'_{K2101+}$ | $M_{K2201+}$ | $M'_{K2201+}$ | $M_{K2301+}$ | $M'_{K2301+}$ | $M_{K1001+}$ | $M'_{K1001+}$ | $M_{K1101+}$ | $M'_{K1101+}$ | $M_{K1201+}$ | $M'_{K1201+}$ |
| 0   | 21      | 0       |         |         |         |         |         |         |         |         |         |         |         |         |
| 2   | 306     | 1       | 327     | 1       | 177     | 0       | 34      | 0       | 124     | 1       | 222     | 0       | 122     | 0       |
| 4   | 2,325   | 7       | 4,662   | 12      | 2,562   | 4       | 504     | 1       | 1,744   | 5       | 3,312   | 7       | 1,732   | 4       |
| 6   | 12,480  | 34      | 34,065  | 90      | 18,815  | 42      | 3,730   | 9       | 12,536  | 36      | 22,533  | 56      | 12,483  | 31      |
| 8   | 52,893  | 144     | 172,500 | 442     | 95,500  | 422     | 19,000  | 46      | 62,540  | 170     | 112,470 | 291     | 62,370  | 160     |
| 10  | 187,842 | 509     | 684,886 | 1,535   | 379,635 | 804*    | 75,670  | 145     | 245,204 | 615     | 441,087 | 1077    | 244,737 | 597     |

Table 2.1: Number of six-nucleon antisymmetrical hyperspherical-spin-isospin state for the case $J = 1$, $T = 0$ and $\pi = +$ as function of the grandangular quantum number $K$, the total spin $S$ and the total angular momentum $L$. $M_{KLSTJ\pi}$ is the total number of antisymmetric states while $M'_{KLSTJ\pi}$ is the number of independent antisymmetric states. With the symbol * we indicate that there are other independent states that must be included to determine the complete basis.
2.4 The variational wave function

The final form of the six-nucleons bound state wave function can be written as

$$\Psi_{6}^{J\pi} = \sum_{l} \sum_{KLST,\alpha} c_{l,\alpha}^{KLST} f_{l}(\rho) \Psi_{\alpha}^{KLST J\pi},$$

(2.61)

where the sum is restricted only on the linear independent antisymmetric states $\alpha$ and $c_{l,\alpha}^{KLST}$ are variational coefficients to be determined. The hyperradial functions $f_{l}(\rho)$ must be chosen in order to satisfy the following criteria: (i) they must constitute a complete basis; (ii) they must satisfy the boundary condition $f(\rho) \to 0$ for $\rho \to \infty$; (iii) their form should be simple but flexible enough to well describe the dependence on the hyperradius. The choice we made is

$$f_{l}(\rho) = \gamma^{D/2} \sqrt{\frac{l!}{(l+D-1)!}} L_{l}^{(D-1)}(\gamma \rho) e^{-\gamma \rho} ,$$

(2.62)

where $L_{l}^{(D-1)}(\gamma \rho)$ are Laguerre polynomials [69] and $\gamma$ is a non-variational parameter that must be determined. A typical range for $\gamma$ is $3.5 - 5.5$ fm$^{-1}$. With such definition, the function $f_{l}(\rho)$ are orthonormal, i.e.

$$\int_{0}^{\infty} d\rho \rho^{D-1} f_{l}(\rho) f_{l'}(\rho) = \delta_{l,l'} .$$

(2.63)

The coefficients $c_{l,\alpha}^{KLST}$ are determined using the Rayleigh-Ritz variational principle. Casting the wave function in the bra-ket notation, Eq. (2.61) becomes

$$|\Psi_{6}^{J\pi}\rangle = \sum_{\xi} c_{\xi} |\Psi_{\xi}\rangle ,$$

(2.64)

where $\xi = \{l, KLST\alpha\}$ and $|\Psi_{\xi}\rangle = f_{l}(\rho) \Psi_{\alpha}^{KLST J\pi}$. Using the Rayleigh-Ritz variational principle, we have

$$\langle \delta c_{6}^{J\pi} | H - E | \Psi_{6}^{J\pi} \rangle = 0 ,$$

(2.65)

where $\delta c_{6}^{J\pi}$ indicates the variation of the wave function for arbitrary infinitesimal changes of the linear coefficients $c_{\xi}$. By performing the variation, the problem is reduced to a generalized eigenvalue problem, where we have to determine the coefficients $c_{\xi}$ and the energy $E$, i.e.

$$\sum_{\xi'} \langle \Psi_{\xi'} | H - E | \Psi_{\xi'} \rangle c_{\xi'} = 0 .$$

(2.66)

Therefore, all the problem stands in calculating the matrix elements of the Hamiltonian $H$ with respect to the basis states. In nuclear physics, the Hamiltonian $H$ is usually given by

$$H = T + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} ,$$

(2.67)

where $T$ is the kinetic energy, $V_{ij}$ the two-body potential and $V_{ijk}$ the three-body potential. In Sections 2.4.1 and 2.4.2 we will discuss the calculation of the kinetic energy and the potential matrix elements, respectively. In this work we will not consider the three-body potential. However, the formalism introduced in Section 2.4.2
can be easily generalized to this case.

Due to the high number of states needed in the expansion to reach convergence, the generalized eigenvalue problem is then solved by using the preconditioned Lanczos method [70], whose main features are presented in Appendix D.

### 2.4.1 Norm and kinetic matrix elements

The first matrix element we need to compute is the norm that multiply the energy $E$, 

$$N_{ξ,ξ'} = \langle \Psi_ξ | \Psi_ξ' \rangle,$$  \hspace{1cm} (2.68)

that explicitly translates into

$$N_{ξ,ξ'} = \int_0^\infty d\rho \rho^{14} \int d\Omega_5 \left[ f_l(\rho) \Psi_{α}^{K'L'S'T'Jπ}(Ω_5) \right]^* f'_l(\rho) \Psi_{α'}^{K'L'S'T'Jπ}(Ω_5).$$  \hspace{1cm} (2.69)

Using the results of Eq. (2.58) and the orthonormal properties of the Laguerre polynomials, we get

$$N_{ξ,ξ'} = N_{KLST Jπ,α,α'}^{KLST Jπ,α,α'} \delta_{KK'} \delta_{LL'} \delta_{SS'} \delta_{TT'} \delta_{ll'}.$$

(2.70)

In the case of the kinetic energy matrix elements, we have

$$T_{ξ,ξ'} = \int_0^\infty d\rho \rho^{14} \int d\Omega_5 \left[ f_l(\rho) \Psi_{α}^{K'L'S'T'Jπ}(Ω_5) \right]^* \hat{T} f'_l(\rho) \Psi_{α'}^{K'L'S'T'Jπ}(Ω_5),$$

(2.71)

where

$$\hat{T} = -\frac{\hbar^2}{m} \left( \frac{\partial^2}{\partial \rho^2} + \frac{14}{\rho} \frac{\partial}{\partial \rho} + \frac{K(K+13)}{\rho^2} \right).$$

(2.72)

The integrals in Eq. (2.71) can be factorized in the hyperradial and hyperangular part, where the last one reduce to Eq. (2.58). The final result is

$$T_{ξ,ξ'} = T_{l,l'} N_{KLST Jπ,α,α'}^{KLST Jπ,α,α'} \delta_{KK'} \delta_{LL'} \delta_{SS'} \delta_{TT'},$$

(2.73)

where

$$T_{l,l'} = -\frac{\hbar^2}{m} \int_0^\infty d\rho \rho^{14} f_l(\rho) \left( \frac{\partial^2}{\partial \rho^2} + \frac{14}{\rho} \frac{\partial}{\partial \rho} + \frac{K(K+13)}{\rho^2} \right) f'_l(\rho),$$

(2.74)

which can be analytically evaluated as shown in Appendix C.1.

### 2.4.2 Potential matrix element

In this section we discuss the calculation of the potential matrix elements, focusing on non-local two-body potentials. The formulas we are presenting here can be easily extended to the calculation of local two-body potentials and three-body potentials.

We need to compute the matrix element

$$V_{KLST, K'L'S'T', Jπ}^{ij,j'} = \left\langle f_l(\rho) \Psi_{α}^{K'L'S'T'Jπ} \left| \frac{1}{2} \sum_{i,j=1}^{A} V_{ij} \langle f_l'(\rho') \Psi_{α'}^{K'L'S'T'Jπ} \rangle \right| \rangle_{Ω,ρ,ρ'} \right. \hspace{1cm} (2.75)$$

where $\Psi_{α}^{K'L'S'T'Jπ}$ is defined in Eq. (2.47), $f_l(\rho)$ is defined in Eq. (2.62) and $\langle \cdots | \cdots \rangle_{Ω,ρ,ρ'}$ denotes the spin and isospin trace and the integration over the hyperspherical and hyperradial variables. The states in the bra and in the ket are totally antisymmetric.
with respect to the exchange of any pair of particles, so it is possible to rewrite the matrix elements in Eq. (2.75) as

$$V_{1a,1a'}^{KLST,K'L'S'T',J\pi} = \frac{A(A-1)}{2} \langle \hat{f}_1(\rho)\psi^{KLSTJ\pi}_\alpha | V_{12} | \hat{f}'_1(\rho')\psi^{K'L'S'T'J\pi}_{1a'} \rangle / \Omega_{\rho,\rho'} \tag{2.76}$$

In order to compute this matrix element it results convenient to use the $jj$-coupling scheme in which the basis state $\alpha$ results

$$\psi^{KLSTJ\pi}_\alpha = \sum_\nu B_{\alpha,\nu}^{KLSTJ\pi} \Xi^{KTJ\pi}_\nu (1, 2, 3, 4, 5, 6), \tag{2.77}$$

where the new transformation coefficients $B_{\alpha,\nu}^{KLSTJ\pi}$ are related to the coefficients $A_{\alpha,\alpha'}^{KLSTJ\pi}$ via 6j- and 9j-Wigner coefficients (see Appendix C.2). The explicit expression for $\Xi^{KTJ\pi}_\nu (1, 2, 3, 4, 5, 6)$ is given by

$$\Xi^{KTJ\pi}_\nu (1, 2, 3, 4, 5, 6) = \mathcal{P}_{n_2,n_3,n_4,n_5}^{l_1,l_2,l_3,l_4} (\varphi_2, \varphi_3, \varphi_4, \varphi_5) \times \left\{ \left( Y_{l_1} (\hat{r}_1) Y_{l_2} (\hat{r}_2) \right) L_2 Y_{l_3} (\hat{r}_3) \left( (s_4 s_5) S_4 S_5 \right) \right\}_{jj} \otimes \left( (t_1 t_2) t_3 t_4 t_5 \right)_{T,T}. \tag{2.78}$$

The index $\nu$ labels all possible choices of the quantum numbers

$$\nu = \{ n_5, l_5, S_2, j_1, n_4, \ell_4, j_2, j_1, \ell_1, \ell_2, \ell_3, L_2, L_3, n_2, n_3, S_4, S_5, j_3, T_2, T_3, T_4, T_5 \}, \tag{2.79}$$

which are compatible with $K, T, J$ and $\pi$. To be noticed that in Eq. (2.78) the $jj$-coupling scheme is used only for the first three particles and all the rest remains in $LS$ scheme. This particular mixed coupling scheme permits to increase the performances of the code which computes the potential matrix elements. Even if in this work we use only two-body forces, this particular coupling scheme results to be very advantageous also when the three-nucleons interaction is included.

The matrix element defined in Eq. (2.76) can be rewritten using the coefficients $B_{\alpha,\nu}^{KLSTJ\pi}$ as

$$V_{1a,1a'}^{KLST,K'L'S'T',J\pi} = 15 \sum_\nu \sum_\nu' B_{\alpha,\nu}^{KLSTJ\pi} B_{\alpha',\nu'}^{K'L'S'T'J\pi} v_{1\nu,1\nu'}^{KT,KT',J\pi}, \tag{2.80}$$

where

$$v_{1\nu,1\nu'}^{KT,KT',J\pi} = \langle \hat{f}_1(\rho)\Xi^{KTJ\pi}_\nu (1, 2, 3, 4, 5, 6) | V_{12} | \hat{f}'_1(\rho')\Xi^{KT'J\pi}_\nu (1, 2, 3, 4, 5, 6) \rangle / \Omega_{\rho,\rho'} \tag{2.81}$$

The quantum numbers $\nu$ can be decomposed as $\nu = \{ \nu_x, \nu_y, T_3 \}$ where

$$\nu_x = \{ j_1, n_4, \ell_4, j_2, j_1, \ell_1, \ell_2, \ell_3, L_2, L_3, n_2, n_3, S_4, S_5, j_3, T_2, T_4, T_5 \}, \tag{2.82}$$

and

$$\nu_y = \{ n_5, \ell_5, S_2 \}. \tag{2.83}$$

Since we consider only parity conserving forces, the potential does not change the
quantum numbers \( j_1 \) and \( T_2 \). Moreover, the potential acts only on the pair \( 1,2 \) without changing the quantum numbers which involves other particles. Therefore, we have that in the matrix element \( \nu_\ell = \nu'_\ell \) and

\[
v_{1\nu_\ell,1\nu'_\ell}^{KT,K'T',J\pi} = \delta_{\nu_\ell,\nu'_\ell} \sum_{T_2z} C_{T_2z,T_3z;J\pi}^{T_2,T_3} v_{K,K',j_1}^{\nu_\ell}(T_{2z}) ,
\]

where

\[
C_{T_2z,T_3z;J\pi}^{T_2,T_3} = \sum_{T_2z} (T_3T_{3z}, T_3z - T_3z|TTz)(T_3T_{3z}, T_3z - T_3z|TTz)
\]

\[
\times (T_2T_{2z}, T_5T_{3z} - T_2z|T_3T_{3z})(T_2T_{2z}, T_5T_{3z} - T_2z|T_3T_{3z}) .
\]

The potential term depends only on the quantum numbers \( K, K', j_1, \nu_\ell, \nu'_\ell \) and the indexes of the Laguerre polynomials \( l \) and \( l' \). Explicitly the potential term reads

\[
v_{1\nu_\ell,1\nu'_\ell}^{\nu_\nu_\nu_\nu}(T_{2z}) = \sum_{\nu_\nu_\nu_\nu} \int_0^\infty dp_5 \int_0^\infty dx_5 (\cos \varphi_5)^{l_5} (\sin \varphi_5)^{l_5} \mathcal{K} \mathcal{P} \nu_\nu_\nu_\nu (x_5) \mathcal{K} \mathcal{P} \nu_\nu_\nu_\nu (x_5) \delta_{S_2, S_2'}
\]

\[
f_{1\nu_\ell,1\nu'_\ell}^{\nu_\nu_\nu_\nu}(T_{2z}) \mathcal{P} \nu_\nu_\nu_\nu (x_5) \mathcal{P} \nu_\nu_\nu_\nu (x_5) \delta_{S_2, S_2'}
\]

where \( \rho^2 = x_5^2 + x_3^2 + x_4^2, \rho' = \rho_5^2 + \rho_3^2, (\rho)^2 = \rho_5^2 + \rho_3^2 \) and \( \cos \varphi_5 = x_5/\rho, \cos \varphi_5 = x_5/\rho' \). Here \( \nu'_{S_2, T_{2z}, j_1}(r, r') \) is the non-local two nucleon potential acting between two-body states \( 2S+1(j) \) and \( 2S+1(j') \) with isospin of the pair \( T_2, T_{2z} \). The three integrals are easily computed numerically with high accuracy with standard quadrature techniques. The final form of the potential matrix element given in Eq. (2.80) is

\[
V_{1\alpha,1\alpha'}^{KLT, J'\pi} = 15 \sum_{\nu} \sum_{\nu'} B_{KLT, J\pi}^{\nu} B_{K'L'S' T', J\pi}^{\nu'}
\]

\[
\times \sum_{T_2z} C_{T_2z,T_3z;J\pi}^{T_2,T_3} v_{1\nu_\ell,1\nu'_\ell}(T_{2z}) \delta_{\nu_\ell,\nu'_\ell} .
\]

### 2.5 Technical details of the calculation

The biggest computational challenge for applying the HH formalism to the \( A = 6 \) system is the calculation and the storage of the potential matrix elements because of the high number of basis states needed to reach convergence. In this section we present the main feature of the algorithm we use to compute the potential matrix elements exploiting the advantages of using the TC. The calculations are performed using a single node with 48 Intel Xenon 8160 CPUs @2.10 GHz.

Before starting to discuss the algorithm, let us give an idea of the dimension of the problem of computing the potential matrix elements in this formalism. We start from Eq. (2.87). The number of operations needed to compute the potential matrix element in Eq. (2.87) is given by \( N_\gamma \times N_{\gamma'} \) where \( N_\gamma (N_{\gamma'}) \) is the total number of TC in \( jj \)-coupling. Once fixed the values of the quantum number \( \gamma = \{K, L, S, T\} \) and \( \gamma' = \{K', L', S', T'\} \) the number of matrix elements we need to compute is \( N_{\gamma} \times N_{\gamma'} \), where \( N_{\gamma} = M_{KLT, J\pi}^{\gamma} \) which is the total number of independent states for given \( \gamma \) as defined in Section 2.3.1. Therefore, fixed \( \gamma \) and \( \gamma' \), the total number
of operations in the computation is given by

$$N_{\text{op}}^{\gamma,\gamma'} \sim N_\gamma \times N_{\gamma'} \times N_\nu \times N_{\nu'}.$$  \hfill (2.88)

If we consider $\gamma = \gamma' = \{12, 2, 1, 0\}$ which is one of the worst cases, we have $N_\gamma = N_{\gamma'} \sim 10^3$ and $N_\nu = N_{\nu'} \sim 2.3 \times 10^6$ then $N_{\text{op}}^{\gamma,\gamma'} \sim 5 \times 10^{18}$. Let us suppose we are in an ideal case in which the time required for any of these operations is the typical clock time of a computer, $10^{-9}$ s, and that we are able to use in parallel $10^3$ CPUs. The total time required for doing all these operations is

$$T_{\text{op}}^{\gamma,\gamma'} \sim 58 \text{ days},$$  \hfill (2.89)

which is a time too long for any practical purpose, especially if we need to repeat these operations for all the possible combinations $\gamma, \gamma'$ and all the potential models we want to study. For this reason we introduce the coefficients $D$, as follows.

As it can be seen from Eq. (2.86), the potential integrals $v_{l
u_y, l'
u'_y}^K K' j_i^j (T_{2z})$ depend only on the index of the Laguerre polynomials and the quantum numbers $T_{2z}$, $K$, $K'$, $j$, $\nu_y$ and $\nu'_y$. Therefore, Eq. (2.87) can be rewritten in a more convenient form as

$$V_{l \alpha, l' \alpha'}^{KLST, K'L'S'T', J \pi} = 15 \sum_{\nu_y} \sum_{T_{2z}} D_{\alpha, \nu_y T_{2z}; l \alpha', l' \nu_y T_{2z}^3}^{KLST, K'L'S'T', J \pi} \sum_{T_{2z}} C_{T_{2z}; T_{2z}}^{T_{2z} T_{2z}^3} \nu_y \nu_y' (T_{2z}) ,$$  \hfill (2.90)

where we denote $D_{\alpha, \nu_y T_{2z}; l \alpha', l' \nu_y T_{2z}^3}^{KLST, K'L'S'T', J \pi}$ the $D$ coefficient and its expression can be easily derived comparing Eq. (2.87) with Eq. (2.90). Explicitly they are given by

$$D_{\alpha, \nu_y T_{2z}; l \alpha', l' \nu_y T_{2z}^3}^{KLST, K'L'S'T', J \pi} = \sum_{\nu_y} B_{\alpha, \nu_y T_{2z}; l \alpha', l' \nu_y T_{2z}^3}^{KLST J \pi} B_{\nu_y, l \nu_y' T_{2z} ; l' \nu_y' T_{2z}^3}^{K'L'S'T', J \pi} \delta_{\nu_y, \nu_y'} .$$  \hfill (2.91)

In this way the only parts which depends on the nuclear interaction in Eq. (2.90) are the potential integrals $v_{l
u_y, l'
u'_y}^K K' j_i^j (T_{2z})$, while the coefficients defined in Eq. (2.91) do not. Therefore, we can compute and store the $D$ coefficients only once for all the potential models we want to consider. However, the time required for the calculation of the $D$ coefficients is still of the order of 50 days.

In order to improve the time consumption, we noticed that for all the possible states $\alpha$ and $\alpha'$ with fixed $\gamma$ and $\gamma'$, the states $\nu$ and $\nu'$ to be coupled are always the same. Therefore, the determination of the couple of states $\nu, \nu'$ that fulfill the $\delta_{\nu_y, \nu_y'}$, which in general requires $N_\nu \times N_{\nu'}$ operations, is performed only once for all the combinations $\alpha, \alpha'$ and requires a typical time of 10–20 minutes for $10 \leq K, K' \leq 14$ using a single node with 48 CPUs working in parallel. The number of operations which remain to be done in Eq. (2.91) is then equal to the number of states $\nu_x (N_{\nu_x})$. In such a way $N_{\text{op}}^{\gamma,\gamma'}$ reduces to

$$N_{\text{op}}^{\gamma,\gamma'} \sim \underbrace{N_\gamma \times N_{\gamma'} \times N_V \times N_{\nu_x}}_{D_{\text{op}}} + \underbrace{N_\nu \times N_{\nu'}}_{\delta_{\nu_y, \nu_y'}} ,$$  \hfill (2.92)

where $N_V$ is the number of combinations $\nu_y, \nu'_y$ permitted by the potential and is typically $< 200$. The $N_{\text{op}}^{\gamma,\gamma'}$ in this case is then orders of magnitude smaller than the value given in Eq. (2.88). Empirically we found that $N_V \times N_{\nu_x} \sim 10 N_\nu$ and considering the optimal computational situation described before, with 1000 CPUs
working in parallel, in the case $\gamma = \gamma' = \{12, 2, 1, 0\}$ we obtain

$$T_{\text{op}}^{\gamma, \gamma'} \sim 23 \text{ s},$$

(2.93)

which is an improvement of $\sim 5$ orders of magnitude. Actually, in a realistic situation, the typical time required for the computation of Eq. (2.91), namely to perform the $N_V \times N_\nu$ operations, is $T_D \sim 0.1$ s. Therefore, for $\gamma = \gamma' = \{12, 2, 1, 0\}$

$$T_{\text{op}}^{\gamma, \gamma'} \sim N_\gamma \times N_{\gamma'} \times T_D \sim 1 \text{ day},$$

(2.94)

where in this case we used only 48 CPUs on a single node. In Figure 2.2 we report the total time needed to compute the $D$ coefficients when $L = L' = 0$, $S = S' = 1$ and $T = T' = 0$ up to given $K = K' = K_{\text{max}}$, namely

$$T_D = \sum_{K=2}^{K_{\text{max}}} \sum_{K'=2}^{K_{\text{max}}} T_{\text{op}}^{K010, K'010}.$$

(2.95)

divided by the number of CPUs ($N_{\text{CPU}}$) used in the computation. In particular, the blue triangles give $T_D$ by using first the pre-identification of the pair of states $\nu, \nu'$ to fulfill the $\delta_{\nu, \nu'}$ condition as discussed before, while the red dots correspond to the time spent without pre-identification. As it is clear from the figure, the computational time increases exponentially by increasing the values of $K_{\text{max}}$, since it is proportional to the number of independent states which grows exponentially as well (see Figure 2.1). However, by using the pre-identification, not only $T_D$ results to be well reduced, but also as function of $K_{\text{max}}$ it has a minor slope compared to the case without pre-identification. The exponential growth limits the maximum value of $K_{\text{max}}$ we can use at present. However, we expect to have a great improvement by using a larger number of CPUs distributing the calculation on several nodes.

As regarding the storage, the total memory required fixed $\gamma$ and $\gamma'$ is given by the number of $D$ coefficient for each $\alpha, \alpha'$ combination, namely

$$M_{\gamma, \gamma'}[\text{GB}] \sim 3 \times \frac{8 \times N_\gamma \times N_{\gamma'} \times N_V}{1024^3},$$

(2.96)

where the factor 3 is an empirical factor which takes care of the additional information needed in the files to save the coefficients $D$. For example, when $\gamma = \gamma' = \{12, 2, 1, 0\}$, the size of the file is only 2.2 GB. The total memory we used to store all the $D$ coefficients used for computing the $^6\text{Li}$ ground state in this work is $\sim 100$ GB. Once computed the $D$ coefficients, the time required for the calculation of all the potential matrix elements is of the order of a couple of hours. Indeed we need only to compute the sum over the combinations $\nu_g, \nu'_g$ allowed by the potential ($N_V$), which are very few.

Typically, in the $ab$-$initio$ methods, the potential matrix elements are computed and stored for each potential model. This requires large amount of time and disk space, limiting the number of models that can be used and tested. On the other hand, by using our approach, we are able to save only the $D$ coefficients by eliminating the dependence on the potential models. In this sense, the HH method, in the context of the $ab$-$initio$ approaches, can act as an efficient and precise method for testing various potential models up to $A = 6$. 
Figure 2.2: Total time needed to compute the $D$ coefficients [Eq. (2.95)] as function of $K = K' = K_{\text{max}}$ divided by $N_{\text{CPU}}$, the number of CPUs used in the computation. These calculations are performed for fixed values of the other quantum numbers, in particular $L = L' = 0$, $S = S' = 1$ and $T = T' = 0$. The red dots are the time spent without pre-identification, while the blue triangles are the time spent with pre-identification. The dashed lines are added to guide the eyes. The calculations were performed on a single node with 48 Intel Xeon 8160 CPUs @ 2.10 GHz (i.e. $N_{\text{CPU}} = 48$).
Chapter 3

The $^6$Li ground state within the Hyperspherical Harmonic basis

In this chapter we present the results obtained for the $^6$Li ground state computed as discussed in the previous chapter. The potential models we use and their major features are briefly introduced in Section 3.1. Section 3.2 is dedicated to present the selection of the HH basis states in order to obtain the best description of the $^6$Li wave function. Finally in Section 3.3 we present the convergence of the HH expansion for the binding energy (BE) and the study of the electromagnetic structure of the $^6$Li ground state.

3.1 The nuclear potential

In all *ab-initio* approaches the goal is to derive the properties of nuclei from fundamental theories. In order to do that the nuclear potential that appears in the Hamiltonian must be connected directly to the QCD Lagrangian. As we already discussed in Chapter 1, the $\chi$EFT approach permits to construct an effective Lagrangian constrained by chiral symmetry and to organize it as an expansion in power of the exchanged pion momentum $Q$. From the Lagrangian, by performing a non-relativistic expansion, it is then possible to derive the nuclear potential which can be organized as well in a expansion in power of $Q$. In particular, modern $\chi$EFT potentials start from order $Q^0$, called leading-order (LO), and then continues with the next-to-leading-order (NLO) of order $Q^2$, the next-to-next-to-leading-order (N2LO or NNLO) of order $Q^3$, the next-to-next-to-next-to-leading-order (N3LO) of order $Q^4$, and in some cases they also take into account next-to-next-to-next-to-leading-order (N4LO) terms of order $Q^5$. In the last years, several nuclear potentials have been constructed starting from the $\chi$EFT Lagrangian providing a practical and systematic scheme to derive two and many-nucleon interactions [37, 38]. Moreover, since $\chi$EFT is a low-energy theory, it is needed to introduce a cut-off $\Lambda_C$ in order to regularize the potential. Each term of the potential is multiplied by a LEC which is determined by reproducing $NN$ and three-nucleon data. The values of the LECs clearly will depend on the cut-off $\Lambda_C$ but the observables should not. Therefore, a proof of the validity of the chiral expansion is that, by increasing the chiral order of the expansion, the values of the observables are less and less dependent on the cut-off. In the future we plan to check this fact on $A = 6$ observables.

However, the solution of the $A = 6$ Schrödinger equation with these potentials is very difficult because of the “hard” repulsive core due to the Pauli principle among the quarks confined in the nucleons, which appears for internucleon distance less than 1 fm. In the Schrödinger equation the “hard” core gives rise to short-range correlations. This requires to construct the wave function with a large set of basis
states, in order to reproduce accurately all these correlations. The required basis size is so large for $A = 6$ that results very hard to use “bare” potentials and reach an acceptable convergence. Only recently, using a softer version of the NNLO potential (NNLO$_{\text{opt}}$ [71]) and a huge computational power, an acceptable convergence has been obtained (see Ref. [72]). However, the short-range correlations can be eliminated decoupling high-momentum (short-range) from low-momentum (long-range) physics, by using the Similarity Renormalization Group (SRG) unitary transformation [73]. This transformation suppresses the off-diagonal matrix elements, the ones that connect high-momentum to low-momentum physics, moving the Hamiltonian towards a band-diagonal form. Let us give an example of how the SRG transformation works as reported in Ref. [73]. The initial Hamiltonian $H = T_{\text{rel}} + V$ in the cm reference frame, where $T_{\text{rel}}$ is the relative kinetic energy, is transformed by the unitary operator $U(s)$ according to

$$H_s = U(s)H U^\dagger(s) = T_{\text{rel}} + V_s,$$

(3.1)

where $s$ is the flow parameter and $V_s$ is the evolved potential. $H_s$ evolves following the relation

$$\frac{dH_s}{ds} = [\eta(s), H_s],$$

(3.2)

with

$$\eta(s) = \frac{dU(s)}{ds}U^\dagger(s) = -\eta^\dagger(s).$$

(3.3)

The selection of $\eta(s)$ determines the transformation. Following Ref. [73], we take

$$\eta(s) = [T_{\text{rel}}, H_s].$$

(3.4)

With this choice $T_{\text{rel}}$ results independent on $s$ in Eq. (3.1). For example, using Eq. (3.4), the two-body potential evolves as

$$\frac{dV_s(k, k')}{ds} = -(k^2 - k'^2)V_s(k, k') + \frac{2}{\pi} \int_0^\infty q^2 dq (k^2 + k'^2 - 2q^2)V_s(k, q)V_s(q, k'),$$

(3.5)

where $V_s(k, k')$ is the non-local two-body potential, $k$ is the relative momentum of the two particles and with normalization so that $1 = \frac{2}{\pi} \int |q|^2 |q dq$ in units where $\hbar^2/m = 1$. From Eq. (3.5), if we do not consider the integral part, we obtain

$$V_s(k, k') \propto e^{-(k^2 - k'^2)^2s},$$

(3.6)

from which it is clear that the off-diagonal matrix elements are exponentially suppressed when $s$ increases. The parameter $\Lambda = s^{-1/4}$ provides a measure of the spread of off-diagonal strength. The suppression of off-diagonal matrix elements decrease the size of the HH basis needed for convergence. However, the SRG transformation on two-body forces ($V^A_{ij} = V_s$) induces three-body forces ($V^A_{ijk}(\text{ind})$), the transformation of the three-body forces ($V^A_{ijk}$) induces four-body forces ($V^A_{ijkl}(\text{ind})$) and so on [73], therefore the Hamiltonian we need to diagonalize becomes

$$H_\Lambda = T_{\text{rel}} + \sum_{i<j} V^A_{ij} + \sum_{i<j<k} V^A_{ijk}(\text{ind}) + \sum_{i<j<k} V^A_{ijk} + \ldots,$$

(3.7)

where the dots stands for $n$-body forces with $N > 3$. It has been shown that $(n+1)$-body forces are less important than the $n$-body ones [74]. Therefore we can safely discard the $n$-body forces with $N > 4$. Moreover, in our calculation, we will not
include three-body forces but, in order to minimize their possible effects, we will use values of $\Lambda$ such that our theoretical results will be close to the experimental values. In particular, we choose values of $\Lambda$ so that the calculated binding energy of $^3\text{He}$, $^3\text{H}$ and $^4\text{He}$ (without the inclusion of bare and induced three-nucleon forces) are close to their experimental values. However, by performing this approximations we pay the price of losing the unitarity properties of our solution. In this Thesis, we will consider the N3LO500 chiral potential [75] (where N3LO is the order of chiral expansion and 500 indicates that $\Lambda_C = 500$ MeV) SRG evolved with three different values of the flow parameter $\Lambda = 1.2$, 1.5 and 1.8 fm$^{-1}$, which we will indicate with SRG1.2, SRG1.5 and SRG1.8, respectively.

The wave function we evaluate with these potentials is not the “bare” wave function. Because of the SRG unitary transformation we have that

$$|\psi(s)\rangle = U(s)|\psi_{\text{bare}}\rangle,$$

where $|\psi(s)\rangle$ is the calculated wave function and $|\psi_{\text{bare}}\rangle$ is the “bare” wave function. The mean value of an operator $O$ (we named it “bare”) can be written as

$$\langle O \rangle = \langle \psi_{\text{bare}}|O|\psi_{\text{bare}}\rangle = \langle \psi(s)|O(s)|\psi(s)\rangle,$$

where $O(s) = U(s)OU(s)\dagger$ is the SRG evolved operator. This transformation is not trivial and up to now available only for few simple operators (see for example Ref. [76]). However, it is expected from the previous discussion that the operator $U$ would mainly take into account the short-range correlations between nucleons. It has been argued that long-range operators would not be affected by it, and therefore $O \approx O(s)$ [77]. For example, square radius and electric quadrupole moment operators can be considered as long-range operators. Therefore, for these we will assume that

$$\langle O \rangle \approx \langle \psi(s)|O|\psi(s)\rangle,$$

where we use the “bare” operator instead of the evolved one. The more this approximation is valid, the less will be the dependence on the parameter $s$.

In our study of $^6\text{Li}$, we will use also the chiral potential NNLO$_{\text{sat}}$ [78]. For this potential, the LECs of the two- and three-body interactions are fitted together to reproduce the NN scattering data and also some $A > 2$ nuclear properties, like the binding energies and charge radii of carbon and oxygen isotopes. The chiral potential constructed in such a way results “softer” than the standard chiral potentials, making possible to perform reliable calculations without using the SRG evolution. Even if the NNLO$_{\text{sat}}$ requires three-body forces to reproduce the physical values of the observables, we will not include them in our calculation. Indeed, we will use this potential only as a test for possible future application of the HH method with other “bare” chiral potentials. In the following, we will indicate with NNLO$_{\text{sat}}$(NN) the NNLO$_{\text{sat}}$ interaction used without considering three-body forces.

### 3.2 Selection of the states

The main difficulty of the HH method is the selection of a subset of basis states which permits to have the best description of the nuclear states we consider. Indeed, although the number of independent states is much smaller than the degeneracy of the basis, a brute force approach of the method, that is the inclusion of all the HH-states having $K \leq K_M$ and then increasing $K_M$ until convergence, would be destined to fail. Moreover, as discussed previously, it is very difficult to find all
Chapter 3. The $^6\text{Li}$ ground state within the Hyperspherical Harmonic basis

| $L$ | $S$ | $T$ | $2S+1L$ |
|-----|-----|-----|---------|
| 0   | 1   | 0   | $^3S_1$ |
| 2   | 1   | 0   | $^3D_1$ |
| 2   | 2   | 0   | $^5D_1$ |
| 2   | 3   | 0   | $^7D_1$ |
| 1   | 0   | 0   | $^1P_1$ |
| 1   | 1   | 0   | $^3P_1$ |
| 1   | 2   | 0   | $^5P_1$ |
| 3   | 2   | 0   | $^5F_1$ |
| 3   | 3   | 0   | $^7F_1$ |
| 4   | 3   | 0   | $^7G_1$ |

Table 3.1: LST components of the ground state wave function of $^6\text{Li}$. In the spectroscopic notation the isospin is neglected since we consider $T = 0$ states only.

the linearly independent states already for values of $K \geq 10$, because of the loss of precision in the orthogonalization procedure. For this reason a good selection of a restricted and effective subset of basis state is fundamental. Up to now we are limited to values $K_M \leq 14$ which permits to reach a reasonable convergence only for the SRG evolved and the NNLO$_{sat}$(NN) potentials.

It is convenient to separate the HH functions into classes taking into account their properties and the fact that the convergence rate of each class results to be rather different. The first selection can be done considering the quantity $\ell_{\text{sum}} = \ell_1 + \ell_2 + \ell_3 + \ell_4 + \ell_5$. Indeed, the HH states with large $\ell_{\text{sum}}$ are less important because of the centrifugal barrier. The SRG potential and the NNLO$_{sat}$(NN) are rather soft and so, in our calculation, we can consider only states with $\ell_{\text{sum}} \leq 4$. The second selection can be done considering the number of particles correlated by the HH functions. The nuclear potential favors the two-body correlations, therefore the HH states which depend only on the coordinate of pair of particles would give important contributions, namely the HH states with only $n_5$ and $\ell_5$ not zero. For technical reasons related to the construction of the TC, we are not able to work with classes defined selecting particular values of $n_2 - n_5$. Therefore we use only the criteria on the $\ell_i$ for the class definition. Moreover, we can divide the $^6\text{Li}$ ground state into LST components. The components allowed by the total spin of $^6\text{Li}$ ground state $J^T = 1^+$ are given in Table 3.1. Being the $^6\text{Li}$ ground state an almost pure $T = 0$ state, we do not consider other isospin states.

To study the $^6\text{Li}$ ground state, we find very convenient to chose the classes as described below.

a. Class C1. In this class we include the HH states such that $\ell_{\text{sum}} = 0$, which belong only to the wave component $^3S_1$. This class represents the main component of the $^6\text{Li}$ wave function, and in order to obtain convergence we include states up to $K_{1M} = 14$.

b. Class C2. In this class we include the HH states such that $\ell_5 = 2$ and $\sum_{i=1,4} \ell_i = 0$. This class contains channels belonging to all the $D$ waves and its contribution is fundamental to obtain a bound $^6\text{Li}$. For this class we include states up to $K_{2M} = 12$.

c. Class C3. This class includes all the HH states that belong to $^3S_1$ component with $\ell_{\text{sum}} = 2$. This class contains only many-body correlations. Therefore,
its impact on the binding energy is less significant. For this class we include states up to $K_{3M} = 10$.

d. Class C4. This class includes all the HH states that belong to the $D$ components and are not included in class C2. As class C3, this class contains HH states with $\ell_{\text{sum}} = 2$ and only many-body correlations, therefore we expect a similar convergence. For this class we include states up to $K_{4M} = 10$.

e. Class C5. This class includes all the independent HH states which belong to the $P$ components and are not included in class C2. As class C3, this class contains HH states with $\ell_{\text{sum}} = 2$ and only many-body correlations, therefore we expect a similar convergence. For this class we include states up to $K_{5M} = 10$.

f. Class C6. This class includes all the independent HH states which belong to the $F$ and $G$ components and are not included in class C2. As class C3, this class contains HH states with $\ell_{\text{sum}} = 2$ and only many-body correlations, therefore we expect a similar convergence. For this class we include states up to $K_{6M} = 10$.

The convergence is studied as follows. First, only the states of class C1 with $K \leq K_1$ are included in the expansion and the convergence of the BE is studied as the value of $K_1$ is increased up to $K_{1M}$. Once a satisfactory convergence for the first class is reached, the states of the second class with $K \leq K_2$ are added to the expansion keeping all the states of the class C1 with $K \leq K_{1M}$. The procedure is then repeated for each new class. Our complete calculation includes about 7000 HH states.

### 3.3 Results for the $^6$Li ground state

In this section we report the results obtained for the ground state of $^6$Li. The calculation are performed using the N3LO500-SRG with $\Lambda = 1.2, 1.5, 1.8 \text{ fm}^{-1}$. The Coulomb interaction is included as “bare” (i.e. not SRG evolved). Moreover, we use also the NNLO sat(NN) considering only the two-body forces. In this work we have $\hbar^2/m = 41.47 \text{ MeV fm}^2$ for all the potentials. Moreover, we use $\gamma = 4 \text{ fm}^{-1}$ in the hyperradial functions [see Eq. (2.62)] which is the optimal value for the parameter $\gamma$ in order to reach convergence on the third decimal digit with a number of Laguerre polynomials $l_{\text{max}} = 16$. For all the considered models, when the angular momentum of the pair $j$ is large the NN interaction becomes very weak. Therefore, all the interactions for $j > 6$ are discarded, since their effects are negligible as it was already shown in Ref. [79] for the $\alpha$ particle. In Appendix E we discuss with more detail the selection of the parameters $\gamma$ and $l_{\text{max}}$ and also the validation of our approach by comparing our results with the results obtained with the non-symmetrized HH (NSHH) method in Ref. [80], using a test potential.

This section is divided in two parts. In the first one, Section 3.3.1, we discuss the convergence of the HH expansion in terms of the various classes. In the second part, Section 3.3.2, we examine the electromagnetic static properties of $^6$Li.

#### 3.3.1 Convergence of the HH expansion

We study the convergence as explained in the previous section, and the results presented are arranged accordingly. For example in Table 3.2, the BE reported in a row with a given set of values $K_1, \ldots, K_6$ has been obtained by including in the expansion all the HH functions of class $C_i$ with $K \leq K_i$ $i = 1, \ldots, 6$. 
Chapter 3. The $^6$Li ground state within the Hyperspherical Harmonic basis

Table 3.2: Convergence of $^6$Li binding energies (MeV) corresponding to the inclusion in the wave function of the different classes C1–C6 in which the HH basis has been divided. The SRG-evolved potential N3LO500-SRGA correspond to $\Lambda = 1.2, 1.5$ and 1.8 fm$^{-1}$.

We show also the results for the NNLO$_{sat}$(NN) potential model.

| $K_1$ | $K_2$ | $K_3$ | $K_4$ | $K_5$ | $K_6$ | 1.2 fm$^{-1}$ | 1.5 fm$^{-1}$ | 1.8 fm$^{-1}$ | NNLO$_{sat}$(NN) |
|-------|-------|-------|-------|-------|-------|--------------|--------------|--------------|-----------------|
| 2     |       |       |       |       |       | 24.779       | 22.315       | 17.946       | 9.188           |
| 4     |       |       |       |       |       | 28.606       | 26.779       | 22.656       | 13.712          |
| 6     |       |       |       |       |       | 29.714       | 28.395       | 24.646       | 16.407          |
| 8     |       |       |       |       |       | 30.030       | 28.937       | 25.425       | 17.760          |
| 10    |       |       |       |       |       | 30.150       | 29.159       | 25.781       | 18.398          |
| 12    |       |       |       |       |       | 30.195       | 29.254       | 25.948       | 18.736          |
| 14    |       |       |       |       |       | 30.213       | 29.295       | 26.031       | 18.931          |
| 14    | 2     |       |       |       |       | 30.263       | 29.362       | 26.108       | 18.997          |
| 14    | 4     |       |       |       |       | 30.900       | 30.481       | 27.619       | 20.828          |
| 14    | 6     |       |       |       |       | 31.318       | 31.626       | 29.819       | 24.557          |
| 14    | 8     |       |       |       |       | 31.413       | 32.006       | 30.827       | 26.843          |
| 14    | 10    |       |       |       |       | 31.437       | 32.122       | 31.195       | 27.880          |
| 14    | 12    |       |       |       |       | 31.444       | 32.167       | 31.352       | 28.361          |
| 14    | 12    | 6     |       |       |       | 31.445       | 32.168       | 31.354       | 28.381          |
| 14    | 12    | 8     |       |       |       | 31.477       | 32.210       | 31.396       | 28.425          |
| 14    | 12    | 10    |       |       |       | 31.493       | 32.233       | 31.422       | 28.459          |
| 14    | 12    | 10    | 4     |       |       | 31.501       | 32.245       | 31.437       | 28.467          |
| 14    | 12    | 10    | 6     |       |       | 31.550       | 32.329       | 31.548       | 28.588          |
| 14    | 12    | 10    | 8     |       |       | 31.577       | 32.389       | 31.642       | 28.738          |
| 14    | 12    | 10    | 10    |       |       | 31.586       | 32.412       | 31.689       | 28.832          |
| 14    | 12    | 10    | 10    | 2     |       | 31.658       | 32.533       | 31.836       | 29.079          |
| 14    | 12    | 10    | 10    | 4     |       | 31.710       | 32.631       | 31.970       | 29.394          |
| 14    | 12    | 10    | 10    | 6     |       | 31.728       | 32.677       | 32.047       | 29.629          |
| 14    | 12    | 10    | 10    | 8     |       | 31.735       | 32.699       | 32.093       | 29.771          |
| 14    | 12    | 10    | 10    | 8     | 4     | 31.736       | 32.703       | 32.101       | 29.790          |
| 14    | 12    | 10    | 10    | 8     | 6     | 31.746       | 32.733       | 32.161       | 29.896          |
| 14    | 12    | 10    | 10    | 8     | 8     | 31.750       | 32.751       | 32.209       | 30.008          |
We can now analyze the results in Table 3.2. For the SRG evolved potentials we observe that classes C1 and C2 are the most important and have the slowest convergence. Indeed the largest values of $K$ must be reached. It is evident that increasing the value of the SRG parameter $\Lambda$, the convergence becomes slower. This is due to the “hardness” of the potential that is enhanced when $\Lambda$ is large. Moreover, class C2 becomes less and less significant when $\Lambda$ becomes smaller. This effect is generated by the SRG evolution, which reduces the correlations between the $S$ wave (class C1) and the $D$ waves (class C2), when $\Lambda$ decreases. Even if classes C1 and C2 are the slowest converging classes, they give 98% of the BE. The contribution of classes C3, C4 is very small for all the values of the flow parameters $\Lambda$ and also the convergence is much faster. It is very interesting to observe that for both classes the contribution to the BE depends less on the value of $\Lambda$ compared to that of classes C1 and C2. This gives an indication that the many-body correlations are not very important for the SRG evolved potentials. We find also that classes C5, which corresponds to $P$ waves, and C6, which corresponds to $F$ and $G$ waves, give a very small contributions to the ground state of the $^6$Li. Moreover, also the convergence is very fast: in order to obtain the same convergence of the other classes, we can stop for $K_{5M} = K_{6M} = 8$.

For the NNLO$_{\text{sat}}$(NN), even if class C1 gives still the main contribution to the BE, its convergence results faster than the convergence of class C2, which indicates the prominence of the $D$ waves in the case of this potential. Indeed, the contribution of the $D$ waves results almost 1/3 of the total BE. Together, classes C1 and C2 give 94% of the total BE. It is clear, comparing the columns of Table 3.2 for these classes with the ones of the SRG cases, that we are not able to reach the same convergence of the SRG potentials. Also classes C3 and C4 result to have a slower convergence compare to the SRG potentials. However their contribution to the BE does not increase dramatically as in the case of class C2. This indicates that also for NNLO$_{\text{sat}}$(NN) many-body correlations are much less important. The $P$ waves (class C5) instead result to be more significant for the NNLO$_{\text{sat}}$(NN) than for the SRG potentials. Indeed, not only its contribution to the BE is almost 1 MeV, but also the convergence rate is slower compared to the SRG case, indicating a stronger correlation of the $P$ waves with the $S$ and $D$ waves. Also in the case of class C6 the contribution to the BE is larger compared to SRG potentials which indicates a relevant presence of $F$ and $G$ waves for this potential.

Let us comment about the convergence rate of the expansion as function of the maximum grand angular quantum number $K_{iM}$ of the various classes of HH states included in our expansion. As shown in various studies [68, 81–83], the convergence of the HH functions towards the exact BE depends primarily on the form of the potential. For the chiral potentials, it was observed empirically that the convergence rate has an exponential behavior as $K_{iM}$ increases. We expect that the same rate of the convergence is obtained also for the SRG evolved potentials as already observed for example in Ref. [74].

To study the convergence behavior, we indicate with $B(K_1, K_2, K_3, K_4, K_5, K_6)$ the BE obtained by including in the expansion all the HH states of class C1 with $K \leq K_1$, all the HH states of class C2 having $K \leq K_2$ and so on. Let us define

$$
\Delta_1(K) = B(K, K_{2M}, 0, K_{4M}, K_{5M}, K_{6M}) - B(K - 2, K_{2M}, 0, K_{4M}, K_{5M}, K_{6M}),
$$

(3.11)

$$
\Delta_2(K) = B(K_{1M}, K, K_{3M}, 0, K_{5M}, K_{6M}) - B(K_{1M}, K - 2, K_{3M}, 0, K_{5M}, K_{6M}),
$$

(3.12)
\[ \Delta_3(K) = B(K_{1M}, K_{2M}, K, K_{4M}, K_{5M}, K_{6M}) - B(K_{1M}, K_{2M}, K - 2, K_{4M}, K_{5M}, K_{6M}), \quad (3.13) \]
\[ \Delta_4(K) = B(K_{1M}, K_{2M}, K_{3M}, K, K_{5M}, K_{6M}) - B(K_{1M}, K_{2M}, K - 2, K_{5M}, K_{6M}), \quad (3.14) \]
\[ \Delta_5(K) = B(K_{1M}, K_{2M}, K_{3M}, K_{4M}, K_{6M}) - B(K_{1M}, K_{2M}, K_{3M}, K_{4M}, K_{5M}, K), \quad (3.15) \]
\[ \Delta_6(K) = B(K_{1M}, K_{2M}, K_{3M}, K_{4M}, K_{5M}, K_{6M}) - B(K_{1M}, K_{2M}, K_{3M}, K_{4M}, K_{5M}, K - 2), \quad (3.16) \]

where with \( K_{iM} \) we indicate that, for the class \( Ci \), we are including all the HH states up to the maximum \( K \) considered in this work. With these definitions, we can compute the “missing” energy for each class due to the truncation of the expansion up to a given \( K_{iM} \), by taking care of the modification of the convergence of a class \( Ci \) due to the inclusion of the other classes. To be noticed that for \( \Delta_1(\Delta_2) \) we put \( K_3 = 0(K_4 = 0) \). This is because the HH states included in class C3(C4) cannot be added to the basis without adding before class C1(C2) due to the orthogonalization procedure. For example, we cannot add the HH states of class C3 with \( K_3 = 6 \) without adding before the HH states of class C1 with \( K_1 = 6 \). Therefore, to have a clear convergence pattern for class C1(C2), we studied it without adding class C3(C4). The changes in the convergence pattern of class C1(C2) due to the coupling with the class C3(C4) are in any case negligible, since class C3(C4) gives a very small contribution to the total BE.

In Figure 3.1 we plot the values of \( \Delta_1, \Delta_2 \) and \( \Delta_5 \) for the four potential models considered. By inspecting the figure, we can see a clear exponential decreasing behavior of the \( \Delta_i \) as function of \( K \), even if the values of \( K \) we used are rather small. In particular, we can assume for each class that
\[ B_i(K) = B_i(\infty) + a_i e^{-b_iK}, \quad (3.17) \]
where \( B_i(\infty) \) is the asymptotic BE of the class \( Ci \) for \( K \to \infty \), while \( a_i \) and \( b_i \) are parameters which depend on the potential and on the class of the HH functions we are studying. In particular, the parameter \( b_i \) indicates the convergence rate of the class \( Ci \). From Eq. (3.17) we obtain
\[ \Delta_i(K) = a_i e^{-b_iK} \left( 1 - e^{2b_i} \right), \quad (3.18) \]
which is used for fitting \( \Delta_i(K) \). The results of the fits are the dashed lines in Figure 3.1. By observing Figs. 3.1a–3.1c in which we study the SRG evolved potentials, it is clear that the convergence rate diminishes by increasing the values of \( \Lambda \). It is also interesting to observe that for \( \Lambda = 1.2 \text{ fm}^{-1} \) we have \( \Delta_1(K) > \Delta_2(K) \), for \( \Lambda = 1.5 \text{ fm}^{-1} \) we have \( \Delta_1(K) \approx \Delta_2(K) \) while for \( \Lambda = 1.8 \text{ fm}^{-1} \) we have \( \Delta_1(K) < \Delta_2(K) \), which confirms the increasing importance of the tensor term of the potential which correlates the \( S \) and \( D \) waves by increasing \( \Lambda \). Moreover, for all the values of the flow parameter \( \Lambda \), we find \( \Delta_5(K) < \Delta_1(K), \Delta_2(K) \), confirming the small contribution of the \( P \) waves to the BE. For the NNLO$_{so}(NN)$ (Fig. 3.1d) we find a situation very similar to the case of \( \Lambda = 1.8 \text{ fm}^{-1} \) in which we have \( \Delta_1(K) < \Delta_2(K) \), even if in this case the convergence is much slower. Also the \( P \) waves (class C5) result to have a more important role in this case, as demonstrate by the fact that from the fit \( \Delta_5(K) \approx \Delta_1(K) \) when \( K = 14 \).

This effects can be seen also by comparing the values of \( b_i \) obtained by the
fits and reported in Table 3.3. For classes C1, C2 and C5 in the case of the SRG evolved potentials, the values of $b_i$ decrease when $\Lambda$ grows. This indicates a more and more repulsive core of the potential when $\Lambda$ increases. Even smaller values of $b_i$ are obtained for the NNLO$_{sat}$\,(NN) potential since it has stronger short-range correlations.

For the classes C3, C4 and C6, the calculated values of $\Delta_i(K)$ are not enough to perform a fit and so we extract the parameter $b_i$ by using only the last two values of $\Delta_i$, namely

$$\frac{\Delta_i(K_iM - 2)}{\Delta_i(K_iM)} = e^{2b_i}. \tag{3.19}$$

This formula gives only a rough estimate of the convergence rate. Therefore, we cannot compare the values of $b_i$ for different potentials. The obtained values of $b_i$ are reported in Table 3.3 as well, except for the class C6 in the cases of NNLO$_{sat}$\,(NN) potential for which the extrapolation was not possible. We will take care of it by considering larger errors on the extrapolations.

Before discussing the calculation of the “missing” energy, we want to underline that Eq. (3.18) represents the asymptotic behavior of the convergence pattern when $K$ is large, while we are using value of $\Delta_i$ computed for not so large values of $K$. For this reason, for the final fit of class C1 and C2 we used only $\Delta_i(K)$ with $K \geq 8$. Indeed, in Figure 3.1 it is possible to observe that, for $K \leq 4$, $\Delta_i$ deviates from the fit. This is usual for the convergence of HH states, as already observed in the case of the $\alpha$ particle in Ref. [79], and is due to the fact that for small values of $K$ the number of states are not enough to give a good description of the wave function.
Chapter 3. The $^6\text{Li}$ ground state within the Hyperspherical Harmonic basis

The “missing” BE due to the truncation of the expansion for each class to finite values of $K = K_{iM}$ can be defined as in Ref. [79]

$$ (\Delta B)_i = \sum_{K=K_{iM}+2,K_{iM}+4,...} \Delta_i(K), \quad (3.20) $$

and by using Eq. (3.18) we obtain

$$ (\Delta B)_i = \Delta_i(K_{iM}) \frac{1}{e^{2b_i} - 1}. \quad (3.21) $$

The “total missing” BE is then computed as

$$ (\Delta B)_T = \sum_{i=1,6} \Delta_i(K_{iM}) \frac{1}{e^{2b_i} - 1}. \quad (3.22) $$

In Table 3.3 we summarize the “missing” BE of each class and the “total missing” BE. By inspecting the table we observe that the “total missing” BE is less than 1% of the total BE for the SRG evolved potential and of the order of 3% for the NNLO$_{\text{sat}}$(NN). This confirms the high accuracy of the computed binding energies. The estimate of the “total missing” BE suffers from the fact that the extrapolation is not really done for large $K$, in particular for the class C3, C4 and C6.

As regarding the errors on the “missing” BE ($\delta(\Delta B)_i$), in the case of the class C1, C2 and C5 we propagate the errors on $b_i$ evaluated in the fits, while for the class C3, C4 and C6 we consider a conservative error of $\delta(\Delta B)_i/(\Delta B)_i = 0.5$. For the class C6, in the case of the SRG1.8, for which we are not able to extrapolate a reliable value of $b_i$, and NNLO$_{\text{sat}}$(NN) potentials, for which we are not able to estimate $b_i$, we consider a more conservative error of $\delta(\Delta B)_i = (\Delta B)_i$. The error on the “total missing” BE is then computed as

$$ \delta(\Delta B)_T = \sqrt{\sum_{i=1,6} (\delta(\Delta B)_i)^2} \quad (3.23) $$

For all the potential considered, the relative error $\delta(\Delta B)_T/(\Delta B)_T$ is of the order of $\sim 15 - 30\%$.

In Table 3.4 we report the computed BE, the extrapolated “exact” BE and a series of other observables associated with the wave function, such as the mean values of the kinetic $\langle K \rangle$ and the potential $\langle V \rangle$ energy, the percentage of $P$, $D$, $F$ and $G$ states, as well as the percentage of the $S = 0, 1, 2, 3$ total spin components. As we already observed, the percentage of $D$ states increases when $\Lambda$ increases and it is almost 8.5% in the case of the NNLO$_{\text{sat}}$(NN). Moreover, for every potential model, the $^6\text{Li}$ ground state turns out to be an almost pure ($> 93\%$) $S = 1$ state.

In order to determine if the computed $^6\text{Li}$ wave function describes a bound nucleus, we need to compare the “exact” BE with the energy of the $\alpha + d$ system $B_{\alpha+d} = B_{\alpha} + B_{d}$ where $B_{\alpha}$ and $B_{d}$ are the BE of the $\alpha$-particle and the deuteron computed with the same potentials (see Chapter 4 for details). For all the interactions considered, we have found $^6\text{Li}$ bound since $B_{\text{extr}} - B_{\alpha+d} > 0$. However, the experimental value $(B - B_{\alpha+d})_{\text{exp}} = 1.4743$ MeV [84] is not very well reproduced by any potential model, very likely because we are not including three-nucleon forces. By comparing the values reported in Table 3.2 with $B_{\alpha+d}$, it is clear that for the SRG evolved potentials the $S$ and $D$ states are sufficient to construct a $^6\text{Li}$ bound of more than 1 MeV. For the case of the NNLO$_{\text{sat}}$(NN) the $P$ waves seem to play
Chapter 3. The $^6$Li ground state within the Hyperspherical Harmonic basis

| $i$ | $K_{iM}$ | $\Delta_i(K_{iM})$ | $b_i$ | $(\Delta B)_i$ | $\Delta_i(K_{iM})$ | $b_i$ | $(\Delta B)_i$ |
|---|---|---|---|---|---|---|---|
| 1 | 14 | 0.013 | 0.51 | 0.007(0) | 0.023 | 0.49 | 0.014(0) |
| 2 | 12 | 0.008 | 0.68 | 0.003(1) | 0.042 | 0.58 | 0.019(0) |
| 3 | 10 | 0.015 | 0.37 | 0.014(7) | 0.022 | 0.32 | 0.024(12) |
| 4 | 10 | 0.008 | 0.60 | 0.004(2) | 0.022 | 0.49 | 0.013(6) |
| 5 | 8 | 0.007 | 0.52 | 0.004(0) | 0.023 | 0.37 | 0.021(0) |
| 6 | 8 | 0.004 | 0.44 | 0.003(1) | 0.018 | 0.26 | 0.026(13) |
| \(\Delta B\)_T | 0.034(7) | \(\Delta B\)_T | 0.117(19) |

| $i$ | $K_{iM}$ | $\Delta_i(K_{iM})$ | $b_i$ | $(\Delta B)_i$ | $\Delta_i(K_{iM})$ | $b_i$ | $(\Delta B)_i$ |
|---|---|---|---|---|---|---|---|
| 1 | 14 | 0.035 | 0.46 | 0.023(0) | 0.074 | 0.43 | 0.05(0) |
| 2 | 12 | 0.144 | 0.50 | 0.084(11) | 0.411 | 0.42 | 0.32(1) |
| 3 | 10 | 0.024 | 0.30 | 0.029(15) | 0.031 | 0.17 | 0.07(4) |
| 4 | 10 | 0.045 | 0.38 | 0.039(20) | 0.093 | 0.25 | 0.14(7) |
| 5 | 8 | 0.049 | 0.26 | 0.070(1) | 0.153 | 0.18 | 0.35(14) |
| 6 | 8 | 0.048 | 0.11 | 0.19(5) | 0.112 | – | – |
| \(\Delta B\)_T | 0.43(9) | \(\Delta B\)_T | 0.93(20) |

Table 3.3: Increments of the $^6$Li BE $\Delta_i(K_{iM})$, computed using Eqs. (3.11)–(3.15) for the various classes $i = 1, \ldots, 6$ and the N3LO500-SRG and NNLO\textsubscript{sat}(NN) potentials. The coefficients $b_i$ are fitted on the $\Delta_i(K)$ for the classes $i = 1, 2, 5$ and computed as in Eq. (3.19) for the classes $i = 3, 4$ and 6. $(\Delta B)_i$ is computed as in Eq. (3.20) and it represents the “missing” BE of each class due to the truncation of the expansion up to a given $K_{iM}$. Finally, the “total missing” BE $(\Delta B)_T$ is computed from Eq. (3.22). Between the parenthesis we report the errors. With (0) we indicate that the errors are smaller than the precision of the digits reported in the table.
Chapter 3. The $^6$Li ground state within the Hyperspherical Harmonic basis

|                     | SRG1.2 | SRG1.5 | SRG1.8 | NNLO$_{sat}$(NN) | Exp.  |
|---------------------|--------|--------|--------|------------------|-------|
| $B$                 | 31.75  | 32.75  | 32.21  | 30.01            | 31.99 |
| $B_{extr.}$         | 31.78(1) | 32.87(2) | 32.64(9) | 30.93(20)       |       |
| $B_s$               | 3.00(1) | 2.46(2) | 2.02(9) | 2.11(20)        | 1.47  |
| $\langle K \rangle$ | 68.67  | 77.68  | 82.55  | 89.62            |       |
| $\langle V \rangle$ | $-100.42$ | $-110.43$ | $-114.76$ | $-119.63$       |       |
| $P_D$               | 3.03   | 4.68   | 6.61   | 8.81             |       |
| $P_P$               | 0.76   | 1.23   | 1.51   | 2.64             |       |
| $P_C$               | 0.01   | 0.03   | 0.05   | 0.11             |       |
| $P_{S=0}$           | 0.65   | 1.02   | 1.22   | 2.03             |       |
| $P_{S=1}$           | 98.53  | 97.32  | 96.06  | 93.64            |       |
| $P_{S=2}$           | 0.51   | 0.99   | 1.59   | 2.60             |       |
| $P_{S=3}$           | 0.31   | 0.66   | 1.12   | 1.73             |       |

Table 3.4: The $^6$Li binding energy ($B$), the extrapolated binding energy ($B_{extr.}$) and the separation energy $B_s = B_{extr} - B_\alpha - B_d$ with the error computed as in Eq. (3.22) (errors on $B_\alpha$ and $B_d$ are not relevant - see Chapter 4), the kinetic ($\langle K \rangle$) and the potential ($\langle V \rangle$) energy for various potential models used in this work. All these quantities are given in units of MeV. Moreover, we report also the percentage of components corresponding to the different waves and of $S = 0, 1, 2, 3$ total spin states of $^6$Li. In the last column we report the available experimental values.

a more important role in the determination of the $^6$Li binding energy. However, since for the NNLO$_{sat}$ potential two- and three-body forces were fitted together, we cannot discuss the role of the different partial waves in determining if the $^6$Li is bound or not, using only the NN part of the interaction. In Table 3.5 we compare our results with those of Ref. [74], obtained using the NCSM. As it can be observed by inspecting the table, the results obtained with the same N3LO-SRGA potentials in Ref. [74], seem to be systematically larger, especially for the case $\Lambda = 1.8$ fm$^{-1}$. The explanation can be found in the fact that the SRG evolution of the N3LO500 potential is slightly different and that the Coulomb potential is included in the SRG evolution [85]. We can exclude that our underbinding is related to errors in our expansion, since we validated it by comparing the results with the ones in Ref. [80] and obtaining exactly the same values with a test potential (see Appendix E). In any case, the present results are in a reasonable agreement with those of Ref. [74], especially considering that they are obtained using two completely different computational techniques.

Finally, we note that no potential model, since we are not including the three-nucleon interactions, is able to reproduce the experimental value of the BE, $B_{exp} = 31.99$ MeV. However, in the case of SRG1.2 and SRG1.8, the probable cancellation between the induced and the “pure” three-body forces, drives the calculated BE closer to the experimental one.

3.3.2 Electromagnetic static properties

In this section we report of the calculated values of the charge radius, magnetic dipole moment and electric quadrupole moment of $^6$Li. The study of these observables allows for a better understanding of the structure of $^6$Li. For the SRG evolved
Chapter 3. The $^6$Li ground state within the Hyperspherical Harmonic basis

This work  | Ref. [74]
---|---
SRG1.2  | 31.78(1) 31.85(3)
SRG1.5  | 32.87(2) 33.00(5)
SRG1.8  | 32.64(9) 32.8(1)
NNLO$_{sat}$(NN)  | 30.93(20) –

Table 3.5: Comparison of the $^6$Li binding energy calculated here with the extrapolated values of Ref. [74], obtained with the NCSM basis up to $N_{max} = 10$. This corresponds to a smaller basis compared to the one used in this work.

\[
\sqrt{\langle R^2_p \rangle} \text{ [fm]} = 0.8751 \\
\langle R^2_n \rangle \text{ [fm]} = -0.1161 \\
hc / \text{MeV fm} = 197.327 \\
m_p c^2 / \text{MeV} = 938.272 \\
\mu_p / \mu_N = 2.7928 \\
\mu_n / \mu_N = -1.9130
\]

Table 3.6: Recommended values from evaluation of experimental data of the various quantities appearing in Eq. (3.24) and (3.30) as obtained from Ref. [88]. We have indicated with $\mu_N$ the nuclear magneton.

potentials, we use the approximation given in Eq. (3.10). Moreover, we discuss the convergence of these observables as function of $K$. In this section with $K$ we indicate the fact that for each class we include all the HH states with $K_i < K$. When $K > K_{iM}$ for a given class $Ci$, this means that we include HH states of this class up to $K_{iM}$.

Charge radius

The mean square (ms) charge radius of a nucleus is given by [86]

\[
\langle r_c^2 \rangle = \langle r_p^2 \rangle + \langle R_p^2 \rangle + \frac{N}{Z} \langle R_n^2 \rangle + \frac{3h^2}{2m_p c^2},
\]

(3.24)

where $\langle R_p^2 \rangle$ and $\langle R_n^2 \rangle$ are the ms charge radii of proton and neutron respectively, and $\frac{3h^2}{2m_p c^2}$ is the Darwin-Foldy relativistic correction [87]. The values used in this work for these three terms are summarized in Table 3.6. The expression in Eq. (3.24) does not include the contribution of spin-orbit terms and meson-exchange currents. The ms value of the proton point radius $\langle r_p^2 \rangle$ is computed as

\[
\langle r_p^2 \rangle = \langle \Psi_{6\text{Li}} | \hat{r}_p^2 | \Psi_{6\text{Li}} \rangle,
\]

(3.25)

where the operator $\hat{r}_p^2$ is defined as

\[
\hat{r}_p^2 = \frac{1}{Z} \sum_{i=1}^{A} (r_i - R_{cm})^2 \left( \frac{1 + \tau_z(i)}{2} \right),
\]

(3.26)
Chapter 3. The $^6$Li ground state within the Hyperspherical Harmonic basis

2.1

2.2

2.3

2.4

2.5

$\hat{r}_p^2 = \frac{1}{6} \sum_{i=1}^{6} (r_i - R_{\text{cm}})^2 = \frac{\rho^2}{12}$. (3.28)

The explicit remaining calculation is discussed in Appendix F.1. In Figure 3.2 we plot the values of the root mean square charge radius $r_c = \sqrt{\langle r_c^2 \rangle}$ as function of $K$. From the figure we can observe for the SRG evolved potentials an exponential behavior as $K$ increases. In order to extrapolate the full converged value, we fit our results with

\[ r_c(K) = r_c(\infty) + ae^{-bK}, \] (3.29)

where $r_c(\infty)$ is the extrapolated value for $K \to \infty$. From the fit we exclude the values of $r_c$ obtained for $K = 2$ and $K = 14$, since they do not follow the exponential behavior, as it can be seen in Figure 3.2. This is due to the fact that for $K = 2$ there are not enough states to well define the structure of $^6$Li, and among the states with $K = 14$ we are not considering channels with $D$ states which are fundamental for describing properly the $^6$Li radius. In Table 3.7 we report the value of the charge radius for the various values of $K$, and the extrapolated one for the SRG evolved potentials in the last row. The error reported in parentheses is due to our fitting procedure. As it can be seen from Table 3.7 and Figure 3.2, the convergence is
Chapter 3. The $^6$Li ground state within the Hyperspherical Harmonic basis

Table 3.7: Charge radii as function of $K$ for the various potential models considered. In the last row we report the extrapolated values for the SRG evolved potentials with the errors (between parenthesis) obtained from the fits of Eq. (3.29). All the values are given in fm.

| $K$ | SRG1.2 | SRG1.5 | SRG1.8 | NNLO$_{sat}$(NN) |
|-----|--------|--------|--------|------------------|
| 2   | 2.233  | 2.138  | 2.133  | 2.165            |
| 4   | 2.267  | 2.150  | 2.117  | 2.098            |
| 6   | 2.338  | 2.217  | 2.168  | 2.109            |
| 8   | 2.386  | 2.274  | 2.223  | 2.151            |
| 10  | 2.417  | 2.313  | 2.267  | 2.196            |
| 12  | 2.433  | 2.337  | 2.298  | 2.233            |
| 14  | 2.440  | 2.346  | 2.307  | 2.240            |
| $r_c(\infty)$ | 2.47(1) | 2.42(2) | 2.52(10) | –                |

Quite slow. Indeed, the HH basis is a “compact” basis and it is not able to describe perfectly the tail of the wave function, which in the case of $^6$Li has a $\alpha + d$ dominant structure, very hard to be reproduced. We will treat this point with more details in Chapter 4. By looking at the results obtained with the SRG potentials, it is clear that the convergence rate is faster for the smallest values of the parameter $\Lambda$, since in these cases the correlations between the nucleons are reduced, favoring the convergence.

As regarding the NNLO$_{sat}$(NN) potential, the convergence is even slower than the SRG evolved potentials and does not show a clear exponential behavior. Therefore, in Table 3.7 we report only our calculations without the extrapolation. Since the NNLO$_{sat}$(NN) potential is less attractive than the SRG evolved ones, we can speculate that $r_c(\infty)$ will be larger. We also expect that by including three-body forces, since they are attractive, this will induce a more compact structure for $^6$Li by reducing the charge radius.

The magnetic dipole moment

The magnetic dipole moment operator for the $A = 6$ case is defined as

\[
\hat{\mu}_z = \mu_p \sum_{i=1}^{6} \sigma_z(i) \left( \frac{1 + \tau_z(i)}{2} \right) + \mu_n \sum_{i=1}^{6} \sigma_z(i) \left( \frac{1 - \tau_z(i)}{2} \right) + \sum_{i=1}^{6} \ell_z(i) \left( \frac{1 + \tau_z(i)}{2} \right),
\]

where $\mu_p$ and $\mu_n$ are the proton and neutron intrinsic magnetic moment, given in Table 3.6, $\sigma_z(i)$ are the Pauli matrices and $\ell_z(i) = (r_i \times p_i)_z$ is the orbital angular momentum of a single particle. We consider the operator projected along the $z$-axis since measurements are performed polarizing the nucleus along such axis. As for the charge radius case, the terms proportional to $\tau_z(i)$ do not contribute. Defining the total spin as

\[
\hat{S}_z = \frac{1}{2} \sum_{i=1}^{6} \sigma_z(i),
\]

the magnetic dipole moment operator becomes

\[
\hat{\mu}_z = \mu_p \sum_{i=1}^{6} \sigma_z(i) \left( \frac{1 + \tau_z(i)}{2} \right) + \mu_n \sum_{i=1}^{6} \sigma_z(i) \left( \frac{1 - \tau_z(i)}{2} \right).
\]
Chapter 3. The $^6\text{Li}$ ground state within the Hyperspherical Harmonic basis

Table 3.8: Values of the magnetic dipole moment as function of $K$ for the various potential models considered. All values are given in units of $\mu_N$.

| $K$ | SRG1.2 | SRG1.5 | SRG1.8 | NNLO$_{sat}$(NN) |
|-----|--------|--------|--------|------------------|
| 2   | 0.872  | 0.868  | 0.866  | 0.862            |
| 4   | 0.864  | 0.858  | 0.852  | 0.846            |
| 6   | 0.864  | 0.857  | 0.850  | 0.840            |
| 8   | 0.864  | 0.857  | 0.850  | 0.840            |
| 10  | 0.864  | 0.858  | 0.851  | 0.843            |
| 12  | 0.864  | 0.858  | 0.852  | 0.845            |
| 14  | 0.865  | 0.858  | 0.852  | 0.845            |

Table 3.8: Values of the magnetic dipole moment as function of $K$ for the various potential models considered. All values are given in units of $\mu_N$.

and the total angular momentum as

$$\hat{L}_z = \sum_{i=1}^{6} \ell_z(i),$$

we can rewrite the magnetic dipole moment as

$$\hat{\mu}_z = (\mu_p + \mu_n)\hat{S}_z + \frac{1}{2}\hat{L}_z.$$

By definition, the mean value of the magnetic dipole moment of $^6\text{Li}$ is given by

$$\langle \mu_z \rangle = \langle \Psi_{^6\text{Li}}(J_z = +1)|\hat{\mu}_z|\Psi_{^6\text{Li}}(J_z = +1) \rangle,$$

where the wave function of $^6\text{Li}$ is in the maximum total angular momentum projection. Analogously we can define the mean values of $\hat{S}_z$ and $\hat{L}_z$, which explicitly reads

$$\langle S_z \rangle = P_{01} + \frac{1}{2}P_{11} + \frac{3}{2}P_{12} - \frac{1}{2}P_{21} + \frac{1}{2}P_{22} + 2P_{23} - P_{32} + \frac{1}{2}P_{33} - \frac{3}{2}P_{34},$$

$$\langle L_z \rangle = P_{10} + \frac{1}{2}P_{11} + \frac{3}{2}P_{12} + \frac{3}{2}P_{21} + \frac{1}{2}P_{22} - P_{23} + 2P_{32} + \frac{1}{2}P_{33} + \frac{5}{2}P_{34}.$$

where $P_{LS}$ is the percentage of the $^{2S+1}L$ partial wave component in $^6\text{Li}$ wave function. The derivation of these formulas is reported in Appendix F.2.

In Table 3.8 and Figure 3.3 we report the results obtained for the various potentials from $K = 2$ to $K = 14$. As it can be seen by inspecting the table, the values of the magnetic dipole moment are practically at convergence. This is due to the fact that the percentages of the different wave components are very stable starting already from $K = 6$. For the SRG potentials, the value of the magnetic dipole moment decreases by increasing the value of $\Lambda$. Indeed, when $\Lambda$ increases the correlations induced by the nuclear potential are stronger, generating a larger amount of $^3D_1$ component in the wave function, which is the only relevant negative component in Eq. (3.35). In the case of the NNLO$_{sat}$(NN) potentials, this effect is even more important, giving a smaller value of the magnetic dipole moment.

If we consider $^6\text{Li}$ to be formed as a $\alpha + d$ cluster, we can expect that

$$\mu_z(^6\text{Li}) \approx \mu_z(d),$$
because the $\alpha$-particle has no magnetic dipole moment. However, the internal structure of $^6\text{Li}$ plays a fundamental role decreasing the value of the magnetic dipole moment compared to the deuteron one, as it can be observed comparing the experimental values (last row of Table 3.9). For this reason, a good potential model should be able to reproduce the differences between the magnetic dipole moments of $d$ and $^6\text{Li}$. In Table 3.9 we compare the results of the magnetic dipole moment of $^6\text{Li}$ and $d$ evaluated with SRG potentials for the three values of $\Lambda$ and the one computed with NNLO$_{sat}$(NN). In all the cases, the $^6\text{Li}$ magnetic dipole moment is reduced compared to the $d$ ones, showing that the potential models are going in the right direction, even if they are not able to reproduce the experimental value. Obviously this is partially due to the fact we are not considering the evolved operator in the SRG case and also that we are not including three-body forces in both the SRG evolved and NNLO$_{sat}$(NN) potentials. However, as it was shown in Refs. [89, 90] for $^3\text{H}$ and $^3\text{He}$, the magnetic dipole moment receives important contributions from two-body electromagnetic currents. We expect that similar corrections are necessary to reproduce the experimental value of $\mu_z(^6\text{Li})$.

|        | $\mu_z(d)$ | $\mu_z(^6\text{Li})$ |
|--------|------------|----------------------|
| SRG1.2 | 0.872      | 0.865                |
| SRG1.5 | 0.868      | 0.858                |
| SRG1.8 | 0.865      | 0.852                |
| NNLO$_{sat}$(NN) | 0.860 | 0.845                |
| Exp.   | 0.857      | 0.822                |

Table 3.9: Values of the magnetic dipole moment of $^6\text{Li}$ and $d$ evaluated with the various considered potential models. In the last row the experimental values are listed [91]. All the values are given in units of $\mu_N$. 

Figure 3.3: Values of the magnetic dipole moment as function of $K$, for three different SRG potential 1.2(blue), 1.5(red), 1.8(green) and the NNLO$_{sat}$(NN) (black).
Electric quadrupole moment

The electric quadrupole moment operator is defined as

$$\hat{Q} = \sum_{i=1}^{6} (3z_i^2 - r_i^2) \left( \frac{1 + \tau_z(i)}{2} \right).$$

Therefore, we can write the mean value as

$$\langle Q \rangle = \langle \Psi_{6Li}(J_z = +1) | \hat{Q} | \Psi_{6Li}(J_z = +1) \rangle,$$  

(3.39)

where the wave function of $^6Li$ is evaluated in the maximum projection of the total angular momentum $J_z = +1$ since the measurements are performed by polarizing the nuclei along the $z$-axis. Again, in Eq. (3.39) the term proportional to $\tau_z(i)$ does not give any contribution as shown in Eq. (3.27). By taking advantage of the antisymmetry of the wave function, the calculation of the mean value of $\hat{Q}$ is reduced to the calculation of the mean value of the operator

$$\hat{Q}(6) = 3 \times (3z_6^2 - r_6^2),$$

(3.40)

where with 6 we indicate that it acts only on the sixth particle. In order to write in a simple form the $\hat{Q}(6)$ operator in terms of the HH states, we define a new set of Jacobi vectors, hereafter denoted as “Q” set, such that

$$\begin{align*}
x_{Q1} &= x_5, & x_{Q2} &= x_2, & x_{Q3} &= x_3, & x_{Q4} &= x_4, & x_{Q5} &= x_1,
\end{align*}$$

(3.41)

and the hyperangular variables $\varphi Q$ as

$$\cos \varphi_i^Q = \frac{x_{Qi}}{\sqrt{(x_{Q1})^2 + \cdots + (x_{Q5})^2}}, \quad i = 2, \ldots, 5,$$

(3.42)

while the definition of $\rho$ does not change. Using these hyperangular variables the operator in Eq. (3.40) can be rewritten as

$$\hat{Q}(6) = 2\sqrt{5\pi} \rho^2 \cos \varphi_5^Q Y_{20}(\hat{x}_5^Q).$$

(3.43)

The use of the “Q” set of hyperspherical variables permits to reduce drastically the number of HH states coupled by the electric quadrupole moment operator in Eq. (3.39), reducing in this way the computational time. The explicit calculation of the electric quadrupole moment in terms of the HH states is given in Appendix F.3.

The study of this observable is crucial for understanding the accuracy of the wave function we computed. Indeed, from the experiment, we know that the electric quadrupole moment of $^6Li$ is very small and negative. For this reason it is challenging for all the potential models to reproduce this value. In Table 3.10 and in Figure 3.4 we report the values of the electric quadrupole moment as function of $K$ for the potential models considered in this Thesis. As it can be observed by inspecting the table and the figure, the trend is irregular up to $K = 8$, and this is due to the cancellations among the contributions coming from different sets of HH states. After $K = 8$, the behavior becomes stable and the convergence very fast since the cancellations are smaller.

The values obtained for the SRG potentials seem to be quite dependent on the value of the parameter $\Lambda$. This is due to the fact we are using the bare operator
Table 3.10: Values of the electric quadrupole moment varying $K$ for SRG potentials with $\Lambda = 1.2, 1.5$ and 1.8 fm$^{-1}$ and for the NNLO$_{sat}$(NN) model. All the values are given in unit of $e$ fm$^2$.

| $K$ | SRG1.2 | SRG1.5 | SRG1.8 | NNLO$_{sat}$(NN) |
|-----|--------|--------|--------|------------------|
| 2   | −0.188 | −0.162 | −0.173 | −0.115           |
| 4   | −0.212 | −0.132 | −0.091 | +0.065           |
| 6   | −0.170 | −0.066 | −0.016 | +0.136           |
| 8   | −0.184 | −0.094 | −0.052 | +0.086           |
| 10  | −0.191 | −0.101 | −0.055 | +0.079           |
| 12  | −0.191 | −0.101 | −0.055 | +0.069           |
| 14  | −0.191 | −0.101 | −0.055 | +0.068           |

Figure 3.4: Values of the electric quadrupole moment for the potential models SRG1.2 (blue), SRG1.5 (red), SRG1.8 (green) and NNLO$_{sat}$(NN) (black) as function of $K$.

in Eq. (3.39) and not the one transformed by the SRG unitary transformation. Therefore, for the electric quadrupole moment the approximation of Eq. (3.10) is not good at all. However, all the SRG models are able to reproduce a small and negative value for the electric quadrupole moment. In particular, for $\Lambda = 1.5$ and 1.8 fm$^{-1}$ we obtain a value quite close to the experimental measurement $-0.0806(6)$ e fm. This is not the case for NNLO$_{sat}$(NN) potential, for which the electric quadrupole moment results to be positive even if very small. In order to understand why we have these differences between the various models, we report in Table 3.11 the partial wave contributions to this observable. As it can be seen, we have large differences only in the contribution coming from $S - D$ matrix element. In particular the value of this matrix element increases when $\Lambda$ increases and it becomes positive with the NNLO$_{sat}$(NN). Therefore, the value of the quadrupole moment seems directly connected to the strength of the tensor term in the nuclear potential: the more is important, the larger is the value of the electric quadrupole moment. Obviously, we need to consider also that three-body forces are not included. However we do not expect that they will be significant. On the other hand, the corrections of two-body currents could be more significant and necessary to obtain a reliable prediction of
the electric quadrupole moment.

|        | S − D | D − D | P − P | P − D | remaining |
|--------|-------|-------|-------|-------|-----------|
| SRG1.2 | −0.187 | −0.023 | 0.009 | 0.009 | < 0.001   |
| SRG1.5 | −0.102 | −0.023 | 0.014 | 0.010 | < 0.001   |
| SRG1.8 | −0.058 | −0.024 | 0.016 | 0.010 | 0.001     |
| NNLO_{sat}(NN) | 0.049 | −0.018 | 0.023 | 0.011 | 0.003     |

Table 3.11: Partial wave contributions to the electric quadrupole moment of $^6$Li. All the values are given in unit of $e\text{ fm}^2$.

3.3.3 Comparison with literature

In order to compare the electromagnetic static properties of $^6$Li calculated here with the results obtained using other techniques, we report in Table 3.12 our N3LO500-SRG1.5 results compared with the values of Ref. [92], calculated using the CD-B2k potential [35] evolved with SRG $\Lambda = 1.5$ fm$^{-1}$. Also the experimental values are listed. Even if the starting interactions are different, the SRG evolution makes the CD-B2k and the N3LO500 potentials very similar, and therefore we can qualitatively compare the results. As regarding the charge radius, our result is in very good agreement with the result reported in Ref. [92]. The experimental value however is underestimated. The reason can be found in the fact that we are using the bare operator and not the evolved one [see Eq. (3.10)] and we also do not include three-nucleon forces. Comparing our calculation for the magnetic dipole moment at $\Lambda = 1.5$ fm$^{-1}$ with the result reported in Ref. [92] (see Table 3.12), we see that our result is larger and not compatible within the error bar. This is probably due to the different potential used in Ref. [92], the CD-B2k, which presumably induces larger $D$ wave components in the wave function. The electric quadrupole moment result, instead, is quite close to the one reported in Ref. [92], taking into account the relative uncertainty. This is also very close to the experimental value, but, as already discussed, this is just a chance, due to the particular choice of the evolution parameter $\Lambda$.

|        | This work(SRG1.5) | Ref. [92] | Exp. |
|--------|------------------|-----------|------|
| $r_c$ [fm] | 2.42(2)          | 2.40(6)   | 2.540(28) [93] |
| $\mu_z$ [$\mu_N$] | 0.858            | 0.843(6)  | 0.822 [91]    |
| $Q$ [$e\text{ fm}^2$] | -0.101           | -0.066(40) | -0.0806(6) [91] |

Table 3.12: Values of the $^6$Li charge radius, $r_c$, magnetic dipole moment, $\mu_z$, and electric quadrupole moment, $Q$, obtained in this work for the N3LO500-SRG1.5, compared with the results of Ref. [92], obtained with the CDB2k-SRG1.5, and with the experimental values.
Chapter 4

The $^6\text{Li}$ Asymptotic Normalization Coefficient

In this chapter we study the $\alpha + d$ clusterization of $^6\text{Li}$ with the goal of determining the ANC, which is the normalization of the long-range tail of the $^6\text{Li}$ wave function. This quantity plays a fundamental role in the determination of the $\alpha + d \rightarrow ^6\text{Li} + \gamma$ radiative capture cross section since this reaction is peripheral at energies relevant for BBN, and therefore the astrophysical factor is practically determined by the square of the ANC (see for example [94]).

This chapter is organized as follows. In the first section we briefly discuss the calculation of the deuteron and $\alpha$-particle wave functions. In Section 4.2 we formally define the $\alpha + d$ cluster form factor (CFF) and the ANC, discussing the calculation and the results. In Section 4.3 we introduce a different approach for computing the CFF from a differential equation. To perform this calculation we introduce a new technique called “projection” method, which we use to compute the terms of the equation. In the last Section we discuss the results obtained by computing the CFF with the equation derived in Section 4.3, and we compare these results with the one obtained in Section 4.2.

4.1 The deuteron and the $\alpha$-particle wave functions

The first ingredients needed to compute the $\alpha + d$ clusterization are the deuteron and the $\alpha$-particle wave functions. Both of them are obtained by solving the two-bodies and four-bodies Schrödinger equation respectively, by using the variational approach presented in Chapter 2. In this section we discuss only the main features and the results.

The variational deuteron wave function is expressed in term of spherical harmonics, namely

$$\Psi_d(x_1) = \sum_{\ell_d=0,2} u_{\ell_d}(x_1) [Y_{\ell_d}^{\ell_1,\ell_2}(\sigma_1,\sigma_2) S_d^{J_d,J_d} (\tau_1,\tau_2) T_d T_d] ,$$

(4.1)

where $x_1 = r_2 - r_1$. The fact that the deuteron is a $J_d^P = 1^+$ states implies that $\ell_d = 0, 2$ and that the spin $S_d = 1$. By imposing antisymmetry we obtain $T_d = 0$. The radial wave functions $u_{\ell_d}(x_1)$ is expanded as

$$u_{\ell_d}(x_1) = \sum_{\ell_d=0}^{\ell_d_{\text{max}}} c_{\ell_d,l_d} f_{\ell_d}(x_1) ,$$

(4.2)
where \( c_{\ell,d,d} \) are the variational parameters determined by using the Rayleigh-Ritz variational principle, and

\[
\hat{f}_d(x_1) = \gamma_d^2 \sqrt{\frac{l_d!}{(l_d+2)!}} L_{l_d}^{(2)}(\gamma_d x_1) e^{-\frac{l_d^2}{4}}. \tag{4.3}
\]

In this work we use \( \gamma_d = 4 \text{ fm}^{-1} \) and \( p^{\text{max}}_d = 40 \). The potential models N3LO500-SRG and NNLO\textit{sat}(NN) are equivalent in the two-body sector and they must reproduce almost exactly the experimental binding energy of the deuteron (\( B_d \)). In Table 4.1 we report the results for the deuteron obtained with the four potentials used in this Thesis, and we compare them with the experimental value. As it can be seen, all the potentials are able to reproduce at the third decimal digit the deuteron binding energy.

| Potential     | \( B_d \) (MeV) |
|---------------|-----------------|
| SRG1.2        | 2.2248          |
| SRG1.5        | 2.2248          |
| SRG1.8        | 2.2248          |
| NNLO\textit{sat}(NN) | 2.2249          |
| Exp.          | 2.224575        |

Table 4.1: Binding energy of the deuteron computed with the N3LO500-SRG and the NNLO\textit{sat}(NN) potential. In the last row we report for comparison the experimental binding energy.

The \( \alpha \)-particle variational wave function is written as

\[
\Psi_\alpha(x_1, x_2, x_3) = \sum_{l_\alpha=0}^{p^{\text{max}}_\alpha} \sum_{K_\alpha} \sum_{\beta_\alpha} a_{\beta_\alpha,l_\alpha} \hat{f}_\alpha(\rho) \sum_{p=1}^{12} \left\{ J_{3\alpha}^{K_\alpha,L_\alpha}(\Omega_{3\rho}) \right\} \left( \gamma_\alpha L_{l_\alpha}^{(8)}(\gamma_\alpha \rho) e^{-\frac{\gamma_\alpha^2}{4}} \right), \tag{4.4}
\]

where \( x_i \) are the Jacobi vectors as defined in Eq. (2.2) by using \( N = 3 \) and \( a_{\beta_\alpha,l_\alpha} \) are the variational parameters. The hyperradial function are defined to be,

\[
\hat{f}_\alpha(\rho) = \gamma_\alpha^2 \sqrt{\frac{l_\alpha!}{(l_\alpha+8)!}} L_{l_\alpha}^{(8)}(\gamma_\alpha \rho) e^{-\frac{\gamma_\alpha^2}{4}}, \tag{4.5}
\]

where in our calculation we use \( \gamma_\alpha = 4 \text{ fm}^{-1} \) and \( p^{\text{max}}_\alpha = 16 \). The expression of the HH function \( J_{3\alpha}^{K_\alpha,L_\alpha}(\Omega_{3\rho}) \) can be easily derived from Eq. (2.27) and Eq. (2.42) by substituting \( A = 4 \) and \( N = 3 \). Moreover, with \( \beta_\alpha \) we indicate all the quantum numbers needed to define the basis, namely

\[
\beta_\alpha \equiv \{ \ell_1, \ell_2, \ell_3, L_2, L_\alpha, n_{2\alpha}, n_{3\alpha}, S_2, S_3, S_\alpha, T_2, T_3, T_\alpha \}. \tag{4.6}
\]

The \( \alpha \)-particle is a \( J^p_\alpha = 0^+ \) state, therefore \( L_\alpha = S_\alpha \). Moreover we consider only \( T_\alpha = 0 \), since it is mainly a isospin 0 state, and all the other \( T_\alpha \) contributions can be safely neglected [79]. In Eq. (4.4), the permutation \( p = 1 \) corresponds to the order \( (1, 2, 3, 4) \) of the particles. This fact will be exploited later in this chapter. We limit our basis states so that \( \ell_\text{sum} = \ell_1 + \ell_2 + \ell_3 \leq 2 \). States with \( \ell_\text{sum} \geq 4 \) do not give any significant contribution. Unlike the \(^6\text{Li}\), being the number of basis states much smaller, we do not perform any other pre-selection. In Table 4.2 we report the
convergence of the binding energy of the $\alpha$-particle ground state ($B_\alpha$) for the four potentials we used. As it can be seen comparing the binding energy at $K_\alpha = 10$, with the extrapolated value, it is clear that we reached the convergence to 1 keV for the SRG evolved potentials and to 10 keV for NNLO$_{sat}$(NN) potential. For the SRG1.5 and SRG1.8 potentials, the binding energy is very close to the experimental one, presumably due to the cancellation between the pure three-body forces and the induced ones. For the NNLO$_{sat}$(NN) we obtain an underbinding of $\sim 1.7$ MeV, due to the fact that we do not include the three-body forces.

| $K_\alpha$ | SRG1.2 | SRG1.5 | SRG1.8 | NNLO$_{sat}$(NN) |
|-----------|--------|--------|--------|-----------------|
| 0         | 25.524 | 25.896 | 24.122 | 17.906          |
| 2         | 26.352 | 27.450 | 26.490 | 21.459          |
| 4         | 26.543 | 27.999 | 28.178 | 25.609          |
| 6         | 26.555 | 28.172 | 28.364 | 26.391          |
| 8         | 26.556 | 28.179 | 28.396 | 26.562          |
| 10        | 26.557 | 28.180 | 28.402 | 26.597          |
| $\infty$ | 26.557 | 28.181 | 28.403 | 26.606          |
| Exp.      |        |        |        | 28.30           |

Table 4.2: Convergence of the binding energy of the $\alpha$-particle ground state computed with the N3LO500-SRG and the NNLO$_{sat}$(NN) potentials as function of $K_\alpha$. We also report the extrapolated values at $K_\alpha \to \infty$. In the last row we report the experimental binding energy.

### 4.2 The $\alpha + d$ cluster form factor

This section is dedicated to study the $\alpha + d$ clusterization of the $^6\text{Li}$ wave function. We begin by defining the cluster wave function as

$$\Psi^{(L)}_{\alpha+d} = N_{\alpha+d} \mathcal{A} [(\Psi_\alpha \times \Psi_d) S Y_L(\hat{r})] J,$$

where the symbol $\mathcal{A}$ is the antisymmetrization operator, $\Psi_\alpha$ and $\Psi_d$ are the wave functions of the $\alpha$-particle and the deuteron calculated in the previous section and $r$ the distance between the $\alpha$ and $d$ c.m. position. The quantum numbers $L$, $S$ and $J$ are determined by considering that $J^{\pi}_\alpha = 0^+$ and $J^{\pi}_d = 1^+$ and so $S = 1$. Moreover, since we are studying the $^6\text{Li}$ ground state, we consider only the case $J^\pi = 1^+$, therefore only $L = 0$ ($S$-wave) and $L = 2$ ($D$-wave) are possible. The normalization $N_{\alpha+d}$ is chosen in order to have

$$\int_{\Omega_S} d\Omega_S |\Psi^{(L)}_{\alpha+d}| = 1,$$

where we are integrating over the hyperspherical surface $\Omega_S$ with an hyperradius $\rho \to \infty$. This condition corresponds of imposing unit flux at infinite distance. Since we are integrating on a surface with infinite radius, this integral receives contributions only from the asymptotic regions in which the six particles are clusterized in $4 + 2$, which corresponds to $\frac{6!}{4!2!} = 15$ regions. Therefore we obtain

$$N_{\alpha+d} = \frac{1}{\sqrt{15}}.$$
We need also to normalize properly the bound state wave function. For a generic wave function of $A$ nucleons, $\Psi_A$, the normalization is given by

$$\langle \Psi_A | \Psi_A \rangle = \int \prod_{i=1}^{A} dr_i \delta \left( R^A_{\text{c.m.}} - 1 \frac{\sum_{j=1}^{A} r_j}{A} \right) |\Psi_A|^2 = 1, \tag{4.10}$$

where $R^A_{\text{c.m.}}$ is a generic position of the c.m. of the $A$ particles. This result follows since the $\Psi_A$ do not depend on $R^A_{\text{c.m.}}$. We note that from the solution of the eigenvalue problem our wave functions are normalized as

$$\int dx_1 |\Psi_d(x_1)|^2 = 1, \quad \int dx_1 dx_2 dx_3 |\Psi_\alpha(x_1,x_2,x_3)|^2 = 1, \quad \int dx_1 dx_2 dx_3 dx_4 dx_5 |\Psi_{6\text{Li}}(x_1,x_2,x_3,x_4,x_5)|^2 = 1, \tag{4.11}$$

where $x_i$ are the Jacobi coordinates as defined in Eq. (2.2) by using $N = 1$ in the case of the deuteron, $N = 3$ in the case of the $\alpha$-particle and $N = 5$ for the $^6\text{Li}$. By using Eq. (4.10) the norms of $d$, $\alpha$ and $^6\text{Li}$ wave functions result

$$\langle \Psi_\alpha | \Psi_\alpha \rangle = \left( \frac{1}{\sqrt{2}} \right)^3, \tag{4.13}$$

$$\langle \Psi_{6\text{Li}} | \Psi_{6\text{Li}} \rangle = \left( \frac{\sqrt{3}}{4} \right)^3. \tag{4.14}$$

We can now define the $\alpha + d$ cluster form factor (CFF) as

$$\frac{f_L(r)}{r} = \frac{\langle \Psi_{6\text{Li}} | \Psi^{(L)}_{\alpha+d} \rangle}{\langle \Psi_{\alpha} | \Psi_{\alpha} \rangle} \left( \frac{\langle \Psi_{6\text{Li}} | \Psi_{6\text{Li}} \rangle}{\langle \Psi_{\alpha} | \Psi_{\alpha} \rangle} \right)^{1/2}, \tag{4.15}$$

where $f_L(r)$ is the so called reduced CFF. In Eq. (4.15) $\langle \Psi_i | \Psi_i \rangle$ represents the normalization of the wave functions as defined in Eqs. (4.12)-(4.14), $\Psi^{(L)}_{\alpha+d}$ the cluster wave function defined in Eq. (4.7), and $\langle \cdots | \cdots \rangle_r$ the traces over the spin and isospin and integration over the internal variables except the intercluster distance $r$, namely

$$\int_r = \int dr_1 dr_2 dr_3 dr_4 dr_5 dr_6 \delta \left( R^6_{\text{c.m.}} - 1 \frac{\sum_{i=1}^{6} r_i}{6} \right) \delta \left( r - |R^d_{\text{c.m.}} - R^\alpha_{\text{c.m.}}| \right). \tag{4.16}$$

We want to underline that by using this definition, the CFF is not sensitive to the choice of the internal coordinates. Considering the results of Eqs. (4.12)-(4.14) and expressing the integral of Eq. (4.16) in terms of the Jacobi vectors of set “B” given in Eq. (2.5), the $\alpha + d$ CFF reduces to

$$\frac{f_L(r)}{r} = \frac{1}{\sqrt{15}} \left( \frac{\sqrt{6}}{4} \right)^{\frac{1}{2}} \int_0^5 dx_i \delta \left( r - \sqrt{\frac{8}{3} x_i} \right) \Psi_{6\text{Li}}^\dagger A [(\Psi_\alpha \times \Psi_d) \Psi_{6\text{Li}}^\dagger Y_L(\hat{r})]_1. \tag{4.17}$$

If we indicate with $\Psi_\alpha(1,2,3,4)$ the wave function of the $\alpha$-particle constructed as the sum over the 12 even permutations of the particles $(1,2,3,4)$ and with $\Psi_d(5,6)$ the wave function of the deuteron constructed with the particles $(5,6)$, we can
rewrite Eq. (4.17) as

\[
\frac{f_L(r)}{r} = \sqrt{15} \left( \frac{\sqrt{6}}{4} \right)^{3/2} \int \prod_{i=1}^{5} dx_i \delta \left( r - \sqrt{\frac{8}{3} r_{2B}} \right) \times \Psi^{(i)}_{6Li} \left[ (\Psi^{(L)}_{\alpha}(1, 2, 3, 4) \times \Psi_d(5, 6))_1 Y_L(r) \right],
\]

where we used the antisymmetry of the \( \alpha \) wave function to eliminate the antisymmetrization operator \( A \), and we have multiplied for a factor 15 to take care of the fact that the initial function \( \Psi^{(L)}_{\alpha+d} \) contains all the \( 4+2 \) partitions of the six particles. The explicit form of Eq. (4.18) in terms of the HH functions is derived in Appendix G. From the CFF, it is possible to calculate the so-called spectroscopic factor, which is defined as

\[
S_L = \int_0^\infty dr f_L(r)^2,
\]

and it can be interpreted as the percentage of \( \alpha + d \) clusterization in the \( ^6\text{Li} \) wave function.

From the CFF, it is possible to derive also the ANC. In the asymptotic regions where the \( ^6\text{Li} \) is completely clusterized in \( \alpha + d \), the wave function can be written as

\[
\Psi_{6Li}^{(\infty)} = \Psi^{(0)}_{\alpha+d} \frac{T_0(r)}{r} + \Psi^{(2)}_{\alpha+d} \frac{T_2(r)}{r}, \quad r \to \infty.
\]

In these regions, the Schrödinger equation of the six particles can be written as

\[
\left[ H_\alpha + H_d - \frac{\hbar^2}{2m} \nabla^2 + \sum_{i \in \alpha, j \in d} V_{ij} \right] \Psi_{6Li}^{(\infty)} = -B_{6Li} \Psi_{6Li}^{(\infty)},
\]

where \( H_\alpha \) and \( H_d \) are the Hamiltonian of the \( \alpha \)-particle and the deuteron which, acting on \( \Psi_{6Li}^{(\infty)} \), gives the binding energies \( B_\alpha \) and \( B_d \). If we consider the limit in which the intercluster distance goes to infinity, the intercluster interaction reduces to the long range Coulomb interactions between protons, and thus Eq. (4.21) becomes

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + \sum_{i \in \alpha, j \in d} \frac{e^2}{r_{ij}} \left( \frac{1 + \tau_z(i)}{2} \right) \left( \frac{1 + \tau_z(j)}{2} \right) + B_c \right] \Psi_{6Li}(r \to \infty) = 0,
\]

where \( B_c = B_{6Li} - B_\alpha - B_d \) is the cluster binding energy and \( e \) the electric charge. Moreover, in this limit, the Coulomb potential reduces to

\[
\sum_{i \in \alpha, j \in d} \frac{e^2}{r_{ij}} \left( \frac{1 + \tau_z(i)}{2} \right) \left( \frac{1 + \tau_z(j)}{2} \right) \Psi_{6Li}(r \to \infty) \xrightarrow{r \to \infty} \frac{2e^2}{r} \Psi_{6Li}(r \to \infty).
\]

Therefore, Eq. (4.21) results

\[
\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{L(L + 1)}{r^2} + 2e^2 \frac{1}{r} + B_c \right] \mathcal{F}_L(r) = 0, \quad \text{with } L = 0, 2,
\]

where \( \mu = \frac{1}{4} m \) is the reduced mass of the \( \alpha + d \) system. The solution of this equation is the Whittaker function, i.e.

\[
\mathcal{F}_L(r) = W_{-\eta, L+1/2}(2kr).
\]
with \( k = \sqrt{2\mu E_r / h^2} \) and \( \eta = 2e^2 / k^* k \). Therefore, the asymptotic form of the wave function results to be

\[
\Psi_{6\text{Li}}(r \to \infty) = C_0 \frac{W_{-\eta, 1/2}(2kr)}{r} \psi_{\alpha+d}^{(0)} + C_2 \frac{W_{-\eta, 5/2}(2kr)}{r} \psi_{\alpha+d}^{(2)},
\]

where the coefficients \( C_0 \) and \( C_2 \) are the so called ANCs for the \( S \)- and the \( D \)-wave, respectively. By comparing the overlap given in Eq. (4.15) with the asymptotic behavior given in Eq. (4.26) we can identify

\[
\lim_{r \to \infty} f_L(r) = C_L W_{-\eta, L+1/2}(2kr).
\]

Therefore, by defining the ratio

\[
C_L(r) = \frac{f_L(r)}{W_{-\eta, L+1/2}(2kr)},
\]

we get the ANC as

\[
C_L = \lim_{r \to \infty} C_L(r).
\]

### 4.2.1 Results for the \( \alpha + d \) cluster form factor and ANCs

In this section we discuss the results obtained for the \( \alpha + d \) CFF and ANC. In particular we focus on the convergence of the CFF and the ANC as function of the maximum \( K \) used in the expansion of the \( ^6\text{Li} \) wave function. In our calculation we use \( l_{\alpha}^{\text{max}} = 40 \) for the calculation of the deuteron, and \( l_{\alpha}^{\text{max}} = 16 \) and \( K_{\alpha} = 8 \) for the \( \alpha \)-particle. We use the \( \alpha \)-particle computed only up to \( K_{\alpha} = 8 \), since the number of HH states used in the expansion is large enough to have good convergence in the binding energy (see Table 4.2), but at the same time it is small enough to be easily managed in the computation of the CFF.

In Figure 4.1 we plot the \( S \)-wave component of the reduced CFF obtained with the N3LO500-SRG1.5 potential. From the figure, it is clear that the tail of the reduced CFF has not the correct behavior of the Whittaker function (full red line) as predicted in Eq. (4.26). This is due to the limited number of HH states used in the expansion of the \( ^6\text{Li} \) wave function, which are not enough to reproduce the correct asymptotic behavior of the reduced CFF. However, it is also clear that the HH states are slowly constructing the correct asymptotic slope when \( K \) increases. On the other hand, for the short range part \((r < 4 \text{ fm})\) the convergence is fast. Similar comments apply also to the \( D \)-wave component given in Figure 4.2.

In Figures 4.3 and 4.4 we compare the reduced CFF calculated with \( K = 12 \) using the various potentials, for \( S \)- and \( D \)-wave component, respectively. By inspecting the figures, it is clear that the “harder” is the potential, the worse the tail of the CFF is constructed. In fact, for “hard” potentials, the HH states are mainly used to construct the short range correlations, and not the tail. As regarding the short range part of the \( S \)-wave component, it is possible to note the presence of a node which does not depend on the particular potential we use, but is strictly related to the symmetry properties of the \( \alpha + d \) clusterization. In particular, the presence of a node reflects the fact that a lower bound state in the \( \alpha + d \) system exists. However, this bound state results totally symmetric and therefore it is forbidden by the Pauli principle. The results obtained for the \( S \)-wave CFF are consistent with the one reported in Refs. [45, 49, 95, 96]. For the \( D \)-wave, the shapes of the CFF are very similar for the SRG evolved potentials but not for the NNLO\text{sat}(NN). In particular,
Chapter 4. The $^6$Li Asymptotic Normalization Coefficient

Figure 4.1: $S$-wave component of the reduced CFF for different values of $K$ used in the expansion of the $^6$Li wave function. The full red line represents the correct asymptotic behavior of the CFF given by the Whittaker function. These results are obtained with N3LO500-SRG1.5 potential.

Figure 4.2: The same as Figure 4.1, for the $D$-wave component.
Chapter 4. The $^6$Li Asymptotic Normalization Coefficient

### Figure 4.3: Comparison of the S-wave component of the reduced CFF calculated with SRG1.2 (blue), SRG1.5 (red), SRG1.8 (green) and NNLO$_{sat}$ (NN) (black) potentials. The CFF are obtained using the $^6$Li wave function computed with $K = 12$.

In the NNLO$_{sat}$ (NN) case, a node, which is not present in the SRG cases, appears. A similar behavior was found in the GFMC calculation of the CFF, done with the AV18/UIX potential in Refs. [45, 95]. The presence of this node can be related to the strength of the tensor term in the potential, as already discussed in Ref. [97]. This hypothesis is confirmed also by the fact that the node disappears in the case of the SRG evolved potentials, where the impact of tensor forces is reduced. The results for the SRG potentials are perfectly consistent with the ones reported in Refs. [49, 96], obtained for SRG evolved potentials as well.

By using Eq. (4.28), we can extrapolate the ANC. In Figure 4.5 we plot the ratio $C_0 (r)$ for the SRG1.5 potential, as function of the maximum value of $K$ in the expansion of $^6$Li. The ratio $C_0 (r)$ shows a sort of “plateau” around the minimum, from which we can try to estimate the ANC. It is nice to observe that by increasing $K$, the “plateau” is enlarging and slowly converging. Similar results are obtained for $C_2 (r)$. In Table 4.3 we report the values of the ANCs estimated by the “plateau” for all the potentials considered, as function of $K$ ($C_L (K)$). Moreover, we indicate also the energy $B_c$ computed for each $K$, since the Whittaker function depends on it. Obviously, when $B_c < 0$ the Whittaker function is not defined and so the ANC, since the $^6$Li results not bound. From the values of $C_L (K)$ we can extrapolate the asymptotic ANC $C_L (\infty)$ by fitting

$$C_L (K) = C_L (\infty) + Ae^{-bK}.$$  \hspace{1cm} (4.30)

on the calculated $C_L (K)$. In the case of the NNLO$_{sat}$ (NN) we cannot give an extrapolation, since the available $C_L (K)$ are not enough for performing a fit. As regarding the theoretical errors we consider a conservative error on $C_L (\infty)$ defined as

$$\Delta C_L = 0.5 \times |C_L (12) - C_L (\infty)|.$$  \hspace{1cm} (4.31)
Figure 4.4: The same as Figure 4.4 for the $D$-wave component.

Figure 4.5: Function $C_0(r)$ as defined in Eq. (4.28) computed for the N3LO500-SRG1.5 by varying $K$ in the expansion of $^6\text{Li}$ wave function. The result for $K = 2$ and 4 are not present since $B_c < 0$. 

Chapter 4. The $^6\text{Li}$ Asymptotic Normalization Coefficient
Table 4.3: Values of the binding energy $B_c$ in MeV and the ANC $C_0$ and $C_2$ in fm$^{-1/2}$ as function of $K$ for the various potential models considered. In the rows indicated with "∞" we report the extrapolated values with the errors (between parenthesis) obtained with Eq. (4.31). However, these estimates of the ANC are rather uncertain due to the lack of well established "plateau" as shown in Fig. 4.5. So to this extrapolation "error" we should add also a systematic error of uncertain magnitude.

In Figure 4.6 we plot the values of $C_0$ as function of $K$ and the fit performed with Eq. (4.30). A similar result is obtained for $C_2$. By comparing Figures 4.3 and 4.4 with the results in Table 4.3, the differences in the tails of the reduced CFF for the various potentials are not enough to explain the numerical differences in the ANCs. The main reason of the differences between the ANCs must be found in the different binding energy $B_c$ used to compute the Whittaker functions. However, these estimates of the ANC are rather uncertain, due to the lack of well established "plateau", as shown in Figure 4.5. Therefore, to this extrapolation "error" we should add also a systematic error of uncertain magnitude.

From the CFF it is also possible to compute the spectroscopic factor $S_L$. In Table 4.4 we report the values of the spectroscopic factors obtained for the various potentials. We do not report the full convergence pattern obtained by varying $K$, but only the converged digits when $K = 12$. For this quantity the convergence issues are less problematic, being an integral quantity. Independently on the potential used, it results that $^6$Li is clusterized in an $\alpha + d$ system for more than 80%. The differences between the values obtained with the SRG evolved potentials can be due to the fact that the induced and proper three-body forces are not included. Moreover, in the table we compare our results with the calculation of Refs. [45, 95, 96]. The values are similar, even if obtained with different potential models. We want to underline that our calculation of the spectroscopic factor is also in line with the experimental estimate of Ref. [20], based on an optical potential analysis of the data.
Figure 4.6: Values of $C_0$ as function of $K$ for the SRG potential models, SRG1.2 (blue), SRG1.5 (red) and SRG1.8 (green). We report also the fit performed using Eq. (4.30) (dashed lines).

| Method         | Potential | $S_0$  | $S_2$  | $S_0 + S_2$ |
|----------------|-----------|--------|--------|-------------|
| HH (This work) | SRG1.2    | 0.909  | 0.008  | 0.917       |
|                | SRG1.5    | 0.868  | 0.007  | 0.875       |
|                | SRG1.8    | 0.840  | 0.006  | 0.846       |
|                | NNLO$_{sat}$(NN) | 0.805 | 0.002  | 0.807       |
| GFMC (Ref. [95]) | AV18/UIX | 0.82   | 0.021  | 0.84        |
| GFMC (Ref. [45]) | AV18/UIX | –      | –      | 0.87(5)     |
| NCSM (Ref. [96]) | CD-B2k    | 0.822  | 0.006  | 0.828       |
| Exp. (Ref. [20]) | –         | –      | –      | 0.85(4)     |

Table 4.4: Values of the spectroscopic factors for the various potential models considered. In the last rows we compare our results with the most recent values in literature and the experimental one.
4.3 Equation for the cluster form factor

Since the procedure adopted so far results somewhat unsatisfactory, due to the difficult identification of the ‘plateau’, in this section we follow another procedure, based on Ref. [98]. With this approach, we can extrapolate the ANC with greater accuracy.

The $^6\text{Li}$ wave function $\Psi_{6\text{Li}}(J^p = 1^+)$ can be written in terms of a complete basis of 4+2 cluster wave functions, namely

$$\Psi_{6\text{Li}} = \sum_{LSnm} I_{LSnm}(r) \frac{1}{\sqrt{15}} A [(\Psi_4^q \times \Psi_2^m)_S Y_L(\hat{r})]_1,$$  \hspace{1cm} (4.32)

where $\Psi_4^q(\Psi_2^m)$ is a four(two)-body cluster wave function, $n(m)$ indicates that it is an eigenstate of the four(two)-body Hamiltonian with eigenvalue $E_n(E_m)$, namely $H_4\Psi_4^q = E_n\Psi_4^q$ and $H_2\Psi_2^m = E_m\Psi_2^m$. The function $I_{LSnm}(r)$ is the overlap integral, and it is defined as

$$I_{LSnm}(r) = \frac{\langle \Psi_4^q \times \Psi_2^m | Y_L(\hat{r}) \rangle_1}{\langle \Psi_4^q | \Psi_4^q \rangle^{1/2} \langle \Psi_2^m | \Psi_2^m \rangle^{1/2}},$$  \hspace{1cm} (4.33)

where $\langle \cdots | \cdots \rangle_r$ indicates that we are using the integral over the internal coordinates as defined in Eq. (4.16), and we have normalized the overlap with the norm of the wave function as defined in Eq. (4.10). In such a way, if we have $\Psi_4^q = \Psi_\alpha$ and $\Psi_2^m = \Psi_d$, we obtain exactly the definition of the $\alpha + d$ CFF, namely

$$I_{LSad}(r) = \frac{f_L(r)}{r},$$  \hspace{1cm} (4.34)

of Eq. (4.15). The wave function $\Psi_{6\text{Li}}$ is the solution of the six-body Hamiltonian

$$H_6\Psi_{6\text{Li}} = -B_{6\text{Li}}\Psi_{6\text{Li}},$$  \hspace{1cm} (4.35)

where the Hamiltonian $H_6$ can be rewritten in terms of the Hamiltonian of the four-body system, the Hamiltonian of the two-body systems and the Hamiltonian describing the relative motion of the two clusters, i.e.

$$H_6 = H_4 + H_2 - \frac{\hbar^2}{2\mu} \nabla^2 + \sum_{i \in \alpha} \sum_{j \in d} V_{ij}.$$  \hspace{1cm} (4.36)

Inserting Eq. (4.32) in Eq. (4.35), multiplying the left-hand-side by the $\alpha + d$ cluster function $\langle \Psi_{6\text{Li}}^{(L)} |$ defined in Eq. (4.7), and integrating over all the internal variables except the intercluster distance $r$, we obtain the differential equation for the $\alpha + d$ reduced CFF $f_L(r)$, i.e.

$$\left[ -\frac{\hbar^2}{2\mu} \left( \frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} \right) + \frac{2\alpha^2}{r} + B_c \right] f_L(r) + g_L(r) = 0,$$  \hspace{1cm} (4.37)

where $B_c = B_{6\text{Li}} - B_\alpha - B_d$. The function $g_L(r)$ is a source term which results to be

$$g_L(r) = \frac{\langle \Psi_{6\text{Li}} | \left( \sum_{i \in \alpha} \sum_{j \in d} V_{ij} - \frac{2\alpha^2}{r} \right) \Psi_{6\text{Li}}^{(L)} \rangle}{\langle \Psi_d | \Psi_d \rangle \langle \Psi_\alpha | \Psi_\alpha \rangle \langle \Psi_{6\text{Li}} | \Psi_{6\text{Li}} \rangle^{1/2}}.$$  \hspace{1cm} (4.38)

When $r \rightarrow \infty$ the source term $g_L(r) \rightarrow 0$ and we obtain exactly Eq. (4.24) and so the
asymptotic solution coincides with the Whittaker function. In this form, Eq. (4.37) can be solved with high accuracy, using the Numerov method, thus obtaining the correct trend of the $f_L(r)$ for $r \to \infty$ and a more accurate value for the ANC.

4.3.1 The projection of the asymptotic states

The calculation of the source term $g_L(r)$ is quite involved, due to the presence of the cluster wave function $|\Psi_{\alpha+d}^{(L)}\rangle$ which does not allow us to use the properties of the HH states in the computation. In order to restore these properties and simplify the calculation, in this section we introduce a new numerical approach called “projection” method.

Any wave function can be expanded in terms of states given by products of HH functions, spin-isospin states, and functions of the hyperradius, since they form a complete basis. Denoting these states by $|HH_{\mu}\rangle$, let us expand a generic antisymmetric cluster wave function $|\Psi_{A+B}\rangle$ as follows

$$
|\Psi_{A+B}\rangle = \sum_{\mu} c_\mu |HH_{\mu}\rangle,
$$

(4.39)

where $c_\mu$ are coefficients defined by projecting the scattering wave function on the $|HH_{\mu}\rangle$ states, namely

$$
c_\mu = \langle HH_{\mu} | \Psi_{A+B} \rangle,
$$

(4.40)

and the states $|HH_{\mu}\rangle$ are normalized such that $\langle HH_{\mu'} | HH_{\mu} \rangle = \delta_{\mu'\mu}$. By expressing our cluster wave function in such a way, it is then possible to compute the source term in Eq. (4.38), taking advantage of the HH properties and in particular of the TC. This method can be applied in different situations but in this section we will focus only on $A = 6$ considering the $\alpha + d$ cluster wave function given in Eq. (4.7), namely

$$
\Psi_{A+B} = \Psi_{\alpha+d}^{LSJ,\xi} = \frac{1}{\sqrt{15}} \{ \{ \Psi_\alpha(p=1) \times \Psi_d(p=1) \}_S Y_L(\hat{r}) \}_J F(r,\xi) \}
$$

$$
= \frac{1}{\sqrt{15}} \sum_{p=1}^{360} [\{ \{ \Psi_\alpha(i,j,k,l) \times \Psi_d(m,n) \}_S Y_L(\hat{r}) \}_J F(r,\xi),
$$

(4.41)

where $F(r,\xi)$ is a generic intercluster function which depends on $r$ and on other possible quantum numbers designed by $\xi$. Let us define the generic cluster wave function $\Psi_{\alpha+d}^{LSJ,\xi}$ in the reference permutation $p = 1$ (1,2,3,4,5,6), which reads

$$
\Psi_{\alpha+d}^{LSJ,\xi}(p = 1) = \{ \{ \Psi_\alpha(p = 1) \times \Psi_d(p = 1) \}_S Y_L(\hat{r}) \}_J F(r,\xi),
$$

(4.42)

With $\Psi_\alpha(p = 1)$ we indicate the term of the $\alpha$ wave function given in Eq. (4.4) corresponding to the reference permutation $p = 1$ of the particles (1,2,3,4) only, while with $\Psi_d(p = 1)$ we indicate the wave function of the deuteron constructed with the particles 5,6.

As basis for our expansion we will consider the HH functions constructed with the set “B” of the Jacobi coordinates as defined in Eq. (2.5) since they are the natural set for describing $\alpha + d$ clusterization. For the hyperradial part we consider the Laguerre polynomials $f_\ell(\rho)$ as defined in Eq. (2.62). Explicitly, the basis in
which we expand is given by

\[ \Phi_{KLT}(p = 1) = f_l(\rho) \left\{ Y_{KLT} \left[ \left( (\sigma_1 \sigma_2)_{S_1} \sigma_3 \right)_{S_3} \left( (\sigma_4 \sigma_5)_{S_4} \sigma_6 \right)_{S_6} \right] \right\}_J \]

(4.43)

where \( Y_{KLT} \) is the HH function defined in Appendix G, and \( \beta \) is the complete set of quantum numbers which defines the basis state as given in Eq. (2.50). From now on we indicate with overlined indices the quantum numbers which refers to the “projection” basis states. Being this a complete basis on the spatial-spin and isospin space, we can rewrite our cluster wave function as

\[ \Psi_{LSJ,\xi}(p = 1) = \sqrt{\frac{15}{360}} \sum_{\ell=0}^{l_{max}} \sum_{K=0}^{K_{max}} \sum_{LST,\beta} c_{KLT,ST}(LSJ,\xi) \Phi_{KLT}(p = 1) . \]

(4.44)

The equivalence holds exactly only when \( K_{max} \to \infty \) and \( l_{max} \to \infty \). Obviously this is not the case in practical applications, since we are limited in the dimension of the basis we can use. However, we can check the quality of our approximation by looking to the convergence of the observables when we increase \( K_{max} \) and \( l_{max} \). The coefficients of the expansion are defined as

\[ c_{KLT,ST}(LSJ,\xi) = \langle \Phi_{KLT,ST} \rangle \langle p = 1 \rangle |\Psi_{LSJ,\xi}(p = 1)\rangle_{\Omega_B,\rho} , \]

(4.45)

where \( \langle \cdot \cdot \cdot | \cdot \cdot \cdot \rangle_{\Omega_B,\rho} \) represents the integration over all the hypercoordinates “B” and the trace over spins and isospins. Their explicit expression and the details of the calculations are given in Appendix H. We note here that this calculation is rather easy, as both wave functions are constructed with the same permutation. Therefore, the angular integration and the spin-isospin traces can be performed analytically (most of them are just \( \delta \)-functions).

Before concluding this section, we need to remember that the cluster function must be totally antisymmetric, namely

\[ \Psi_{LSJ,\xi}(p = 1) = \frac{1}{\sqrt{15}} \sum_{p=1}^{360} \Psi_{LSJ,\xi}(p) . \]

(4.46)

Let us expand \( \Psi_{LSJ,\xi}(p) \) in terms of the basis states \( \Phi_{KLT,ST}(p) \) constructed with the same permutation. The expansion coefficients in this case are nothing else than the coefficients of Eq. (4.44), as it is easy to prove, redefining the numberings of the particles in order to obtain the reference permutation \((1, 2, 3, 4, 5, 6)\). Thus,

\[ \Psi_{LSJ,\xi}(p = 1) = \sqrt{\frac{15}{360}} \sum_{\ell=0}^{l_{max}} \sum_{K=0}^{K_{max}} \sum_{LST,\beta} c_{KLT,ST}(LSJ,\xi) \Phi_{KLT,ST}(p) , \]

(4.47)

where thanks to the fact that we are using the HH formalism, we can impose antisymmetrization by selecting only the states \( \beta \) such that \((-1)^{\ell_2 + S_2 + T_2} = -1\). Therefore,
expressing the sum over the permutations through the TC, we have

\[
\psi^{LSJ,\xi}_{\alpha+d} = \frac{1}{\sqrt{15}} \sum_{l=0}^{l_{\text{max}}} \sum_{K=0}^{K_{\text{max}}} \sum_{LST,\beta} A^{K_{\text{LST}},B}_{K,\beta} \Phi^{K_{\text{LST}}}(p = 1),
\]

(4.48)

where \(A^{K_{\text{LST}},B}_{K,\beta}\) are the TC computed in the set of coordinates “B” (see Appendix B for more details). We are now ready for computing the source term.

### 4.3.2 Calculation of the Source Term

The source term given in Eq. (4.38) can be divided in a Coulombian term, defined as

\[
g^C_L(r) = -\frac{2e^2}{r} \sqrt{\frac{15}{4}} \int \prod_{i=1}^{5} dx_i B \delta \left( r - \sqrt{\frac{8}{3}} x^2_B \right) \times \psi^6_{\text{Li}} \left[ \sum_{i\in\alpha} \sum_{j\in d} V_{ij} \right] \left[ (\psi_\alpha(1,2,3,4) \times \psi_d(5,6)) Y_L(\hat{r}) \right]_1,
\]

and a potential term, defined as

\[
g^V_L(r) = \sqrt{\frac{15}{4}} \left( \frac{\sqrt{6}}{4} \right)^{\frac{3}{2}} \int \prod_{i=1}^{5} dx_i B \delta \left( r - \sqrt{\frac{8}{3}} x^2_B \right) \times \psi^6_{\text{Li}} \left[ \sum_{i\in\alpha} \sum_{j\in d} V_{ij} \right] \left[ (\psi_\alpha(1,2,3,4) \times \psi_d(5,6)) Y_L(\hat{r}) \right]_1,
\]

(4.50)

where the symbols and the arguments used to derive these expressions are the same as used in Eq. (4.18). In this section, in order to simplify the notations, we consider only local potentials. The generalization to the non-local ones is straightforward.

As regarding the calculation of the Coulomb part, we can repeat the procedure followed for the \(\alpha + d\) CFF in Section 4.2. The computation of the potential part is more involved due to the presence of the \(\delta\)-function. In order to overcome this difficulty, we can expand \(g^V_L(r)/r\) in terms of the Laguerre polynomials, i.e.

\[
g^V_L(r) = \sum_{n=0}^{N_{\text{max}}} C_n^L f_n(r),
\]

(4.51)

where

\[
f_n(r) = \gamma^\frac{3}{2} \sqrt{\frac{n!}{(n+2)!}} L_n^{(2)}(\gamma r) e^{-\gamma r}.
\]

(4.52)

The parameter \(\gamma\) is chosen to optimize the expansion. The coefficients \(C_n^L\) are given by

\[
C_n^L = \int dr r^2 g^V_L(r) f_n(r),
\]

(4.53)
and, substituting Eq. (4.50) in Eq. (4.53), we obtain

\[
C_n^L = \sqrt{15} \left( \frac{\sqrt{6}}{4} \right)^{\frac{3}{2}} \int \prod_{i=1,3} dx_i B \Psi_{6Li} \left( \sum_{i} \sum_{j} V_{ij} \right) \times \left[ \Psi_\alpha(1,2,3,4) \times \Psi_d(5,6) \right] Y_L(\hat{r}) f_n(r) \bigg|_{r=\sqrt{\frac{r}{2}x_B}}.
\]  

(4.54)

We can now define the cluster wave function as

\[
\Phi_{L,n} = \left[ \Psi_\alpha(1,2,3,4) \times \Psi_d(5,6) \right] Y_L(\hat{r}) f_n(r).
\]  

(4.55)

which can be expanded by using the “projection” method. Let us remember that \(\Psi_\alpha(1,2,3,4)\) is built by summing over the 12 even permutations of \((1,2,3,4)\). Therefore, Eq. (4.55), in terms of the “projection” basis states given in Eq. (4.43) reads

\[
\Phi_{L,n} = \sum_{l=0}^{l_{\text{max}}} \sum_{K=0}^{K_{\text{max}}} \sum_{LST,\beta} \sum_{\gamma} \frac{\xi_{LST}}{\xi_{\beta}} \Phi_{LST}(L,n) \sum_{p\alpha=1}^{12} \Phi_{KLST}(p\alpha),
\]  

(4.56)

where with \(p\alpha\) we indicate the even permutation of \((i,j,k,l)\) of the six particles \((i,j,k,l,5,6)\). To be noticed that in this case, contrarily to Eq. (4.48), since we are not summing over all the 360 permutations of the six-particles, the states \(\beta\) are not necessarily antisymmetric. Now let us change the numberings of the particles so that the potential acts always on particles \((1,2)\). In this way Eq. (4.54) reduces to

\[
C_n^L = 4\sqrt{15} \left( \frac{\sqrt{6}}{4} \right)^{\frac{3}{2}} \int \prod_{i=1,3} dx_i B \Psi_{6Li} \left( \sum_{i} \sum_{j} V_{ij} \right) \times \left[ \Psi_\alpha(1,2,3,4) \times \Psi_d(5,6) \right] Y_L(\hat{r}) f_n(r) \bigg|_{r=\sqrt{\frac{r}{2}x_B}}.
\]  

(4.57)

where \(p^*\) are \(12 \times 8 = 96\) even permutations deriving from this operation of reordering (the 96 permutations derive from the \(\sum_{p\alpha}\) and \(\sum_{ij}\)). In order to compute this integral it is convenient to return to the standard set of hypercoordinates. Therefore, we rewrite the sum over permutation \(p^*\) by using the TC, which in \(jj\)-coupling results in

\[
\sum_{p^*} \Phi_{KLST}^{K\beta}(\rho, \Omega_{Bp^*}) = \sum_{B} B_{K\beta,\nu^*}^{KLST,Bs+1} \varepsilon_{\nu^*}^{KLST}(\rho, \Omega_5),
\]  

(4.58)

where the coefficients \(B_{K\beta,\nu^*}^{KLST,Bs+1}\) are computed summing only on the permutations \(p^*\) and transforming the HH functions written in terms of set “B” in terms of the standard one (see Appendix B), while the functions \(\varepsilon_{\nu^*}^{KLST}(\rho, \Omega_5)\) are defined in Eq. (2.78). Finally, the coefficients \(C_n^L\) are given by

\[
C_n^L = 4\sqrt{15} \left( \frac{\sqrt{6}}{4} \right)^{\frac{3}{2}} \int \prod_{i=1,3} dx_i B \Psi_{6Li} \left( \sum_{i} \sum_{j} V_{ij} \right) \times \left[ \Psi_\alpha(1,2,3,4) \times \Psi_d(5,6) \right] Y_L(\hat{r}) f_n(r) \bigg|_{r=\sqrt{\frac{r}{2}x_B}}.
\]  

(4.59)

where \(a_{l_{\alpha}}^{KLST}\) are the variational coefficients of the \(^6\)Li wave function and \(\nu\) is defined
in Eq. (2.79). Here we have used the expansion of $^6\text{Li}$ wave function in terms of the standard set of HH functions. The potential matrix elements $v_{l\nu l'\nu'}^{K,T,K'T'}$ are exactly the ones given in Eq. (2.81) and can be computed by using the same approach of Section 2.4.2. Note that this formula does not depend on the locality/non-locality of the potential, which appears only in the potential matrix elements.

### 4.4 Results

In this section we discuss the results obtained for the $\alpha + d$ CFF by using Eq. (4.37). Furthermore, we compare the CFF obtained with the two methods, i.e. using the direct overlap (Section 4.2) and the equation (Section 4.3).

For the calculation of the source term we use the following parameters. We use $N_{\text{max}} = 20$ for the expansion with the Laguerre polynomials of the potential part of the source term [Eq. (4.51)]. We use $l_{\text{max}} = 40$ for the hyperradial part of the cluster function [Eq. (4.56)]. Both these values permit to reach full convergence in the respective expansions. More difficult results to be the expansion in HH states, as shown by the dependence on $K$. In Table 4.5 we report the total number of HH states used in the projection of both $S$- and $D$-wave components of the cluster wave function for fixed $K, L$ and $S$.

As can be seen by inspecting the table, the number of states grows very fast as function of $K$. This limits our calculation to $K_{\text{max}} = 8$. However, by considering all the projecting states up to $K_{\text{max}} = 8$, we are reproducing completely the hyperangular-spin-isospin structure of the $\alpha$ wave function with our projections, since we use the $\alpha$-particle computed with $K_\alpha = 8$. What remains are the radial part of the deuteron wave function and the hyperradial part of the $\alpha$-particle wave function, which are reproduced by the remaining Jacobi polynomials and the hyperradial functions (see Appendix G.2). Hereafter, in this section, with $K$ we indicate that we are including all the possible states $\beta$ with all the possible $L$, $S$ and $T$ allowed such that $K(\beta) \leq K$.

In Figure 4.7 we plot the reduced source term $g_L(r)$ for the $S$-wave component of the CFF in the case of N3LO500-SRG1.5 potential for different values of $K$. The calculation shown in this plot is performed by considering the $^6\text{Li}$ wave function.

| $L$ | $\bar{S}$ | $K = 0$ | $K = 2$ | $K = 4$ | $K = 6$ | $K = 8$ |
|-----|-----|-----|-----|-----|-----|-----|
|     |     | $S$ | $D$ | $S$ | $D$ | $S$ | $D$ | $S$ | $D$ | $S$ | $D$ |
| 0 1 | 6 0 | 18 0 | 60 12 | 168 60 | 414 228 | 
| 1 0 | 0 0 | 4 0 | 30 8 | 124 68 | 376 292 | 
| 1 1 | 0 0 | 6 0 | 48 18 | 234 162 | 732 672 | 
| 1 2 | 0 0 | 2 0 | 20 10 | 126 80 | 416 362 | 
| 2 1 | 0 0 | 12 6 | 72 48 | 294 252 | 906 936 | 
| 2 2 | 0 0 | 6 0 | 42 12 | 180 100 | 576 452 | 
| 2 3 | 0 0 | 2 0 | 12 2 | 50 20 | 158 100 | 
| 3 2 | 0 0 | 0 0 | 10 10 | 56 72 | 218 304 | 
| 3 3 | 0 0 | 0 0 | 2 2 | 12 16 | 50 72 | 
| 4 3 | 0 0 | 0 0 | 2 2 | 10 12 | 36 46 | 
| Total | 6 0 | 50 6 | 298 124 | 1254 842 | 3882 3464 | 

Table 4.5: Total number of HH states used in the expansion of the $S$- and $D$-wave of the cluster wave functions for given values of $K, L$ and $\bar{S}$.
Chapter 4. The \(^6\)Li Asymptotic Normalization Coefficient

Figure 4.7: \(S\)-wave component of the reduced source term \(g_0(r)\) for different values of \(K\) used in the projection of the \(α + d\) cluster wave function. This figure is obtained by using N3LO500-SRG1.5 potential, and the \(^6\)Li wave function computed with \(K = 12\).

computed for \(K = 12\). From the figure it is immediately clear that we have a nice convergence in \(K\) for the short-range part \((r < 3 − 4 \text{ fm})\) but not for larger \(r\). This effect is due to the fact that the Jacobi polynomials are not flexible enough in reproducing the exponential behavior of the wave function. This means that a larger number of states in the projection are needed to describe correctly \(g_L(r)\) for \(r > 4\) fm. However, by inspecting the figure it results clear that there are problems only in a region where \(g_0(r)\) is a factor 100 smaller than the peak. A similar convergence behavior in \(K\) is founded also for the other potentials studied and for \(g_2(r)\).

Let us now study how these considerations on \(g_L(r)\) are reflected on the CFF calculated via Eq. (4.37). We find that, even if the source term is exponentially decreasing and vanishing for large \(r\), the different behavior of the tail as function of \(K\) has an impact on the ANC, although it is not large. In Figure 4.8 we compare the \(S\)-wave reduced CFF computed using the N3LO500-SRG1.5 potential and the \(^6\)Li wave function with \(K = 12\) for various values of \(K\). As already discussed for the source term, in the region \(r\) below \(3 − 4\) fm we reach full convergence with \(K = 8\). As regarding the tail, thanks to the vanishing term \(g_L(r)\) for larger \(r\), we obtain the Whittaker function which is the correct asymptotic behavior. However its normalization (i.e. the ANC) depends a bit on \(K\) as the tail of \(g_L(r)\). In any case this effect is quite small in particular for the “harder” potentials, as can be seen from the good convergence in \(K\) in Figure 4.8 and in Table 4.6. On the other hand, the \(D\)-wave ANCs result to be more dependent on \(K\).

In Table 4.7 we report the value of the ANC computed with the projection method for \(K = 8\) as function of \(K\) used for computing the \(^6\)Li wave function. Since we can not give a reliable extrapolation for \(K \rightarrow \infty\) due to the fact the convergence pattern is not clear (see Table 4.6) we report also an error given by the half of
**Chapter 4. The $^6$Li Asymptotic Normalization Coefficient**

Figure 4.8: $S$-wave component calculated via Eq. (4.37) of the reduced $\alpha + d$ CFF $f_0(r)$ for different values of the $\overline{K}$ used in the projection of the cluster wave function. For comparison we report also the result obtained with the direct overlap (red line). These results are obtained with N3LO500-SRG1.5 potential and the $^6$Li wave function computed with $K = 12$.

| $\overline{K}$ | SRG1.2 | SRG1.5 | SRG1.8 | NNLO$_{sat}$(NN) |
|----------------|--------|--------|--------|-----------------|
| $C_0$ [fm$^{-1/2}]$ |
| 2 | -7.86 | -6.34 | -5.22 | -4.77 |
| 4 | -4.00 | -3.17 | -2.59 | -2.51 |
| 6 | -4.40 | -3.59 | -2.98 | -2.83 |
| 8 | -4.17 | -3.45 | -2.90 | -2.84 |

| $C_2$ [fm$^{-1/2}]$ |
|----------------|--------|--------|--------|
| 2 | 0.136 | 0.084 | 0.051 | 0.027 |
| 4 | 0.170 | 0.115 | 0.073 | 0.044 |
| 6 | 0.080 | 0.043 | 0.025 | 0.013 |
| 8 | 0.115 | 0.072 | 0.044 | 0.026 |

Table 4.6: Values of the $C_0$ and $C_2$ in fm$^{-1/2}$ as function of $\overline{K}$. All the results given in this table are obtained by considering the $^6$Li wave function computed at $K = 12$. 
difference between the ANC computed for $K = 6$ and $K = 8$, namely
\[
\Delta C_L^{(0)}(K) = 0.5 \times |C_L(K, K = 6) - C_L(K, K = 8)|. \tag{4.60}
\]

By repeating the same procedure used in Section 4.2.1, we fit the values of the ANCs obtained with $K = 8$ for different values of $K$ by using the exponential function given in Eq. (4.30). The extrapolated values for $K \to \infty$ are reported in the last row for each potential. As error due to the extrapolation on $K$, we consider a conservative error estimated as
\[
\Delta C_L^{(1)} = 0.5 \times |C_L(12, K = 8) - C_L(\infty)| \tag{4.61}
\]
and a total error on our final extrapolation of
\[
\Delta C_L = \sqrt{\left(\Delta C_L^{(0)}(12)\right)^2 + \left(\Delta C_L^{(1)}\right)^2}. \tag{4.62}
\]

We can now compare the ratio of the $\alpha + d$ CFF with the Whittaker function obtained with the two methods. In Figure 4.9 we plot the functions $C_0(r)$ defined in Eq. (4.28) obtained with the two methods for two different values of $K$ used for the calculation of the $^6\text{Li}$ wave function. For the equation method we consider the results obtained with $K = 8$. For the SRG potentials it is clear that the short-range part of $C_0(r)$ computed with the two methods are essentially indistinguishable. This is not the case of the tail, since the $C_0(r)$ computed with the direct overlap is not following the correct asymptotic behavior, as already discussed. Moreover, it is possible to observe that, when the potential becomes “harder” as in the case of SRG1.8 and

| $K$ | SRG1.2 | | SRG1.5 | |
|-----|--------|-----|--------|-----|
|     | $B_c$ | $C_0$ | $C_2$ | $B_c$ | $C_0$ | $C_2$ |
| 2   | -3.736 | -     | -     | -7.634 | -     | -     |
| 4   | 0.891  | -3.04(3) | 0.041(1) | -1.615 | -     | -     |
| 6   | 2.359  | -3.74(12) | 0.092(4) | 1.071  | -2.82(8) | 0.029(3) |
| 8   | 2.766  | -4.08(5) | 0.111(13) | 1.929  | -3.30(1) | 0.063(9) |
| 10  | 2.909  | -4.10(12) | 0.114(16) | 2.222  | -3.37(7) | 0.070(13) |
| 12  | 2.955  | -4.17(12) | 0.115(18) | 2.323  | -3.45(7) | 0.072(15) |
| ∞   | 3.00(1) | -4.19(12) | 0.116(18) | 2.46(2) | -3.44(7) | 0.072(15) |

| $K$ | SRG1.8 | | NNLO_{sat}(NN) | |
|-----|--------|-----|----------------|-----|
|     | $B_c$ | $C_0$ | $C_2$ | $B_c$ | $C_0$ | $C_2$ |
| 2   | -12.108 | -     | -     | -18.74 | -     | -     |
| 4   | -5.105  | -     | -     | -10.99 | -     | -     |
| 6   | -0.911  | -     | -     | -4.16  | -     | -     |
| 8   | 0.740   | -2.61(1) | 0.024(4) | -0.74  | -     | -     |
| 10  | 1.332   | -2.80(4) | 0.039(7) | 0.61   | -2.61(1) | 0.015(3) |
| 12  | 1.551   | -2.90(4) | 0.044(10) | 1.15   | -2.83(1) | 0.026(6) |
| ∞   | 2.02(9) | -3.01(7) | 0.047(10) | 2.11(20) | n.a. | n.a. |

Table 4.7: Values of the binding energy $B_c$ in MeV and the ANCs $C_0$ and $C_2$ in fm$^{-1/2}$ as function of $K$ for the various potential models computed using Eq. (4.37). In the row labeled with “∞” we report the extrapolated values. The errors (between parentheses) are obtained with Eq. (4.60) for the various $K$ and with Eq. (4.62) for the extrapolated values.
Chapter 4. The $^6$Li Asymptotic Normalization Coefficient

**Figure 4.9:** Function $C_0(r)$ computed with the overlap method (dashed lines) and the equation method (continuous lines) for all the potential considered. The calculations are performed with the $^6$Li wave function computed with $K = 10$ (blue lines) and $K = 12$ (red lines). Results of the equation method are obtained using $K = 8$.

NNLO$_{sat}$(NN), the differences between the $C_0(r)$ functions computed with the two methods start at smaller values of $r$. For example, in the case of NNLO$_{sat}$(NN) even the short range part does not completely coincide. This effect is directly related to the convergence in both $K$ and in $K$: the better is the convergence in both the expansions, the closer are the results of the two methods. In Figure 4.10 we plot the same for $C_2(r)$. In this case, even if the general shapes result similar, for all the potentials the $C_2(r)$ obtained with the equation method seems systematically larger compared to the one obtained with the direct overlap method. We suppose that such a difference is related to the poor description of the $D$-wave components in the $^6$Li wave function.

In Table 4.8 we compare the extrapolated values of the ANC computed with the two methods. By inspecting the table it is evident that the results obtained with the equation method are systematically larger than the ones obtained in Section 4.2.1. Even if the equation method results are affected by larger errors due to the expansion in the HH states of the cluster wave function, this systematic difference cannot be explained simply giving the responsibility to a not complete convergence in $K$ for the projection of the cluster wave function. Indeed, in the case of the SRG1.2 potential, the convergence in $K$ is almost reached and still this systematic difference persists. As discussed previously, the ANCs directly calculated from the overlap suffer of unknown systematic uncertainties, therefore we consider the ones calculated from the equation as more reliable. For completeness in the table we report also the experimental values of Ref. [99] and the calculation of Refs. [45, 47] obtained using the AV18/UIX and the N3LO500-SRG1.5 with three-body forces, respectively. We can not really perform a comparison, since our results do not contain the contribution
Table 4.8: Values of the extrapolated ANC $C_0$ and $C_2$ in fm$^{-1/2}$ for the various SRG-evolved potential models and the two methods used for the calculation. We report also the binding energy $B_c$ (MeV) used in the calculation of the ANC and the ratio $C_2/C_0$. For completeness we shows also the results of the ab-initio calculation of Refs. [45, 47] obtained with the AV18/UIX potential and the N3LO500-SRG1.5 including three-body forces (3b). Also the experimental values of Ref. [99] are listed.
of the three-body forces, and they are not computed at the physical energy $B_c$. However, from a qualitative point of view, there is a nice agreement since all the SRG potential models used are able to reproduce the correct magnitude of the ANC. This result is quite remarkable, if we consider that the potential models we use are constrained only to nucleon-nucleon data and do not have any information on the $A = 6$ nuclei.
Chapter 5

The \( p + ^6\text{Li} \rightarrow ^7\text{Be} + \gamma \) radiative capture reaction

In this chapter we present a theoretical study of the \( p + ^6\text{Li} \rightarrow ^7\text{Be} + \gamma \) radiative capture reaction within a cluster model. The cluster model approach is based on the fact that the two colliding nuclei can be considered as structureless particles, which interact through an \textit{ad hoc} potential. This approach is completely different from the \textit{ab-initio} approach used in the previous chapters. First of all, here, we are not starting from first principles, therefore the potential model we consider is limited to describe only the \( p - ^6\text{Li} \) system. Moreover, in the \textit{ab-initio} approaches the full \( A \)-body Hamiltonian is solved, while in this chapter we consider a simple two-body Hamiltonian which is a very crude approximation. However, even if this is a quite simple model, it permits to predict the \( S \)-factor and the angular distribution of the emitted photons with a good accuracy.

This chapter is organized as follows. In Section 5.1 we introduce the general formalism of the cluster model approach. In Section 5.2 we present the \( p - ^6\text{Li} \) potential model used in this calculation, while in Section 5.3 we discuss our results. All the results of this chapter have been already published in Ref. [66].

5.1 Theoretical formalism

Let us consider a generic reaction \( A_1 + A_2 \rightarrow A_3 + \gamma \). By considering the nuclei \( A_1 \) and \( A_2 \) as structureless particles, the scattering wave function is written as

\[
\psi_{1,2}(r, p) = \frac{\sqrt{4\pi}}{p} \sum_{LSJJ_3} i^L \sqrt{2L + 1} (J_1 M_1, J_2 M_2|SJ_z)(SJ_z, L0|JJ_z) \psi_{1,2}^{LSJJ_z}(r, p),
\]

with

\[
\psi_{1,2}^{LSJJ_z}(r, p) = R_{LSJ}(r, p) \left[ Y_L(\hat{r}) \otimes \chi_S \right]_{JJ_z},
\]

where \( p \) is the relative momentum of the two particles, \( r \) the intercluster distance, \( L, S \) and \( J \) the total orbital, spin and angular momentum of the system, with \( J_1, M_1 \) and \( J_2, M_2 \) being the total angular momenta and third components of the two nuclei. In Eq. (5.2), \( \chi_S = \left( \phi_{J_1} \phi_{J_2} \right)_S \) is the “spin” state of the two clusters. The function \( R_{LSJ}(r, p) \) is the scattering wave function, that has been determined solving the two-body Schrödinger equation similarly to what has been done in Ref. [31]. For the bound states of the final nucleus \( A_3 \) we write the wave function as

\[
\psi_3^{J_3M_3}(r) = u_{J_3S_3}(r) \left[ Y_{J_3}(\hat{r}) \otimes \chi_{S_3} \right]_{J_3M_3},
\]
where $r$ is again the intercluster distance. The function $u_{L_3S_3}(r)$ has also been determined as explained above. The total cross section for a radiative capture in a bound state with total angular momentum $J_3$ is written as

$$
\sigma_{J_3}(E) = \frac{32\pi^2}{(2J_1 + 1)(2J_2 + 1)} \frac{\alpha}{v_{\text{rel}} 1 + q/m_3} \sum_{A \geq 1} \sum_{LSJ} \left( |E_{LSJ,J_3}^\Lambda|^2 + |M_{LSJ,J_3}^\Lambda|^2 \right),
$$

(5.4)

where $\alpha = e^2/4\pi$, $v_{\text{rel}}$ is the relative velocity of the two incoming particles, $q$ is the photon momentum and $m_3$ is the mass of $A_3$ nucleus. Finally, $T_{\Lambda}^{LSJ,J_3}$, with $T = E/M$, are the reduced matrix element of the electromagnetic operator and $\Lambda$ is the multipole order. Using the Wigner-Eckart theorem, they are defined as

$$
T_{\Lambda}^{LSJ,J_3} = \langle \psi_{1/2}^{LSJJ_{3}}(r, p) | T_{\Lambda}^{LSJJ_{3}}(r) | \psi_{3}^{J_{3}M_{3}}(r) \rangle \sqrt{2J_{3} + 1} \frac{\sqrt{3}}{(J_{3}M_{3}, \Lambda \lambda | JJ_{2})},
$$

(5.5)

where $\lambda = \pm 1$ is the photon polarization. In our calculation we include only the electric multipoles, which are typically much larger than the magnetic ones. Then, in the long-wavelength approximation [100], by using Eqs. (5.2) and (5.3), it results

$$
E_{\Lambda}^{LSJ,J_3} = (-1)^{2J_1 + \Lambda + L + S - J} \hat{J}_{3} \hat{L}_{3} \hat{\Lambda} (L_0, 0, 0 | L_0) \left\{ \begin{array}{ccc} J & L & S \\ L_3 & J_3 & \Lambda \end{array} \right\} \times \frac{Z_e^{(\Lambda)}}{(2\Lambda + 1)!!} \frac{q^\Lambda}{\sqrt{4\pi \pi}} \int_0^\infty dr \, r^2 u_{L_3S_3}(r) r^4 R_{LSJ}(r, p) \delta_{S_3}(r).
$$

(5.6)

Here we have defined $\hat{x} = \sqrt{2x + 1}$ and

$$
Z_e^{(\Lambda)} = Z_1 \left( \frac{m_2}{m_1 + m_2} \right)^\Lambda + Z_2 \left( \frac{m_1}{m_1 + m_2} \right)^\Lambda
$$

(5.7)

is the effective charge, in which $Z_1(Z_2)$ is the charge and $m_1(m_2)$ is the mass of the $A_1(A_2)$ nucleus. Given the radial wave functions $u_{L_3S_3}(r)$ and $R_{LSJ}(r, p)$, the one-dimensional integral of Eq. (5.6) is simple and it can be calculated easily with standard numerical techniques. The astrophysical $S$-factor is then defined as

$$
S_{J_3}(E) = E \exp(2\pi\eta) \sigma_{J_3}(E),
$$

(5.8)

where $\sigma_{J_3}(E)$ is the total cross section for a radiative capture reaction

$$
\sigma_{J_3}(E, \theta) = \sigma_0(E) \sum_{k \geq 0} a_k^{J_3}(E) P_k(\cos \theta),
$$

(5.9)

where $\sigma_0(E)$ is a kinematic factor defined as

$$
\sigma_0(E) = \frac{16\pi^2}{(2J_1 + 1)(2J_2 + 1)} \frac{\alpha}{v_{\text{rel}} 1 + q/m_3},
$$

(5.10)

and $P_k(\cos \theta)$ are the Legendre polynomials. Note that we have defined the $z$-axis as the direction of the incoming protons in the lab, and the $xy$ plane as the plane where the photon is emitted. Since the initial particles are unpolarized and the final polarizations are not measured, the cross section depends only on $\theta$, the angle
between \( p \) and \( q \). The coefficients \( a_k \) are given by

\[
a_{k}^{J_{3}}(E) = \sum_{L'L'S'J'\Lambda'\Lambda} (-)^{J'+J_{3}+L'+\Lambda+\Lambda'} L'L'\Lambda'\Lambda J J' k \left( L_{0} L_{0} | k_{0} \right) \{ L L' k J' J S S' \} \{ L L' k J J' J_{3} \} \sum_{\lambda = \pm 1}^{\Lambda = \pm 1} (\Lambda' - \lambda, \Lambda \lambda | k_{0}) \times \left( \lambda M_{N} L'L'S'J_{3} + E_{N}^{L'L'S'J_{3}} \right) \left( \lambda M_{\Lambda} L'L'S'J_{3} + E_{\Lambda}^{L'L'S'J_{3}} \right)^{*}. \tag{5.11}
\]

The photon angular distribution can be casted in the final form

\[
\sigma_{J_{3}}(E, \theta) = \sigma_{J_{3}}(E) \left( 1 + \sum_{k \geq 1} A_{k}^{J_{3}}(E) P_{k}(\cos \theta) \right), \tag{5.12}
\]

where \( \sigma_{J_{3}}(E) \) is defined in Eq. (5.4), and \( A_{k}^{J_{3}}(E) = a_{k}^{J_{3}}(E)/a_{0}^{J_{3}}(E) \). All these formulas are derived explicitly in Appendix I.

### 5.2 The \( p - ^{6}\text{Li} \) potential model

In our study we consider as clusters the two colliding nuclei, \( p (J^{\pi} = 1/2^{+}) \) and \( ^{6}\text{Li} (J^{\pi} = 1^{+}) \). The potential model we build is tuned to reproduce the \( ^{7}\text{Be} \) properties and the elastic scattering phase shifts. Following Ref. [62], we consider a \( p - ^{6}\text{Li} \) potential of the form

\[
V(r) = -V_{0} \exp \left( -a_{0}r^{2} \right), \tag{5.13}
\]

where \( V_{0} \) and \( a_{0} \) are two parameters to be selected independently for phase-shifts of each different \( L, S, J \) waves. We also add a point-like Coulomb interaction, i.e.

\[
V(r) = \alpha \frac{Z_{1}Z_{2}}{r}, \tag{5.14}
\]

where \( \alpha = 1.439975 \text{ MeV fm} \). All the other coefficients entering the two-body Schrödinger equation solved in this framework are given for completeness in Table 5.1. All the following results have been obtained using the Numerov algorithm to solve the Schrödinger equation and then tested using the R-matrix method (see Ref. [101] and references therein).

| \( m_{p} \) | 1.00727647 u [88] |
| \( m_{\text{Li}} \) | 6.01347746 u [84] |
| \( \hbar c \) | 197.3269788 MeV fm [88] |

**Table 5.1:** Values of the parameters used in the Schrödinger equation obtained. Note that we have used 1 u = 931.4940954 MeV [88].

The parameters of the intercluster potential given in Eq. (5.13) are chosen in order to reproduce the elastic scattering phase shifts, which are derived from partial wave analysis of the experimental elastic scattering data of Ref. [62]. In Table 5.2 we report all possible partial waves up to orbital angular momentum \( L = 2 \) that are needed, both for the doublet \( S = 1/2 \) and quartet \( S = 3/2 \) states, \( S \) being the sum of the proton and \( ^{6}\text{Li} \) spins, 1/2 and 1 respectively. While the value of \( a_{0} \) has been fixed and kept as in Ref. [62], the values of \( V_{0} \) has been obtained minimizing the \( \chi^{2} \)
Chapter 5. The $p+^6\text{Li}\rightarrow^7\text{Be}+\gamma$ radiative capture reaction

Table 5.2: Partial waves of the $p(J^\pi = 1/2^+)-^6\text{Li}(J^\pi = 1^+)$ system up to $L = 2$. We indicate with $S$ the total spin.

| $L$  | $S = 1/2$  | $S = 3/2$  |
|------|-------------|-------------|
| 0    | $^2S_{1/2}$ | $^4S_{3/2}$ |
| 1    | $^2P_{1/2}$, $^2P_{3/2}$ | $^4P_{1/2}$, $^4P_{3/2}$, $^4P_{5/2}$ |
| 2    | $^2D_{3/2}$, $^2D_{5/2}$ | $^4D_{1/2}$, $^4D_{3/2}$, $^4D_{5/2}$, $^4D_{7/2}$ |

\[ \chi^2 = \sum_i \frac{(\delta_i^\text{EXP}(E) - \delta_i^\text{TH}(V_0, E))^2}{(\Delta\delta_i^\text{EXP})^2}. \]  

Here $\delta_i^\text{EXP}(E)$ are the experimental phase shifts and $\delta_i^\text{TH}(V_0, E)$ are the calculated ones. The minimization has been performed using the COBYLA algorithm [102]. The values of $V_0$ and $a_0$ for the various partial waves and the corresponding $\chi^2$/datum are listed in Table 5.3. To be noticed that the phase shift for the $^2P$ wave is given by $\delta_{2P} = \delta_{2P_{1/2}} + \delta_{2P_{3/2}}$ as defined in Ref. [62]. The data set we used from Ref. [62] has no information on the $D$ waves. Therefore, in order to evaluate the $^2D$ and the $^4D$ waves, we use the same potential parameters used for the $^2S_{1/2}$ and $^4S_{3/2}$ respectively, changing only the angular momentum $L$ in the Schrödinger equation. Moreover, we impose that the $D$ waves have the same radial part regardless of $J$.

Table 5.3: Values for the parameters of the Gaussian potential and $\chi^2$/datum for the different partial waves.

| wave | $V_0$ (MeV) | $a_0$ (fm$^{-2}$) | $\chi^2$/datum |
|------|-------------|-----------------|----------------|
| $^2S_{1/2}$ | 124.63 | 0.15 | 0.4 |
| $^4S_{3/2}$ | 141.72 | 0.15 | 3.6 |
| $^2P$ | 67.44 | 0.1 | 1.9 |

The $p-^6\text{Li}$ potential of Eq. (5.13) is used also in order to describe the $^7\text{Be}$ nucleus. In this case we need to reproduce the binding energies of the two bound states, the ground state (GS) $J^\pi = 3/2^-$ with $B = 5.6068$ MeV and the first excited state (FES) $J^\pi = 1/2^-$ with $B = 5.1767$ MeV [84]. We fixed again the parameter $a_0$ as in Ref. [62], while in order to obtain $V_0$ we impose that the calculated binding energies reproduce the experimental ones up to the sixth digit. Moreover, we have evaluated also the ANC, defined in this case as

\[ \text{ANC} = \frac{u_{LS}(r)}{\sqrt{2kW_{L+1/2}(2kr, \eta)}}, \]  

where $u_{LS}(r)$ is the radial part of the wave function [see Eq. (5.3)], $r$ is the inter-cluster distance, $k = \sqrt{\frac{2\mu B}{\hbar^2}}$ with $\mu = \frac{m_p m_{^6\text{Li}}}{m_p + m_{^6\text{Li}}}$, $B$ the binding energy of the bound
Chapter 5. The $p + ^6\text{Li} \rightarrow ^7\text{Be} + \gamma$ radiative capture reaction

5.3 Results

In this section we compare our theoretical predictions for the astrophysical $S$-factor and the angular distribution of the emitted photon with the available experimental data. In the last part, we also discuss the possibility of introducing in our model the resonance proposed in Ref. [59].

Before discussing the results, we note that in the $p - ^6\text{Li}$ reaction the open $^3\text{He} - ^4\text{He}$ channel should in principle be included. However, we do not consider this channel in our work. This can be done, because the experimental phase shifts of Ref. [62] used to fit our potential were obtained considering only the $p - ^6\text{Li}$

\[ J^\pi \quad V_0 \text{ (MeV)} \quad a_0 \text{ (fm}^2) \quad B \text{ (MeV)} \quad \text{ANC} \]

| $J^\pi$ | $V_0$ (MeV) | $a_0$ (fm$^2$) | $B$ (MeV) | ANC  |
|--------|-------------|---------------|-----------|------|
| $3/2^-$ | 254.6876510 | 0.25          | 5.606800  | 2.654|
| $1/2^-$ | 252.7976803 | 0.25          | 5.176700  | 2.528|

Figure 5.1: Phase shifts for the $^2S_{1/2}$ and the $^4S_{3/2}$ partial waves as function of the proton energy. The data are taken from Ref. [62]. The full red line are the calculated phase shifts with the potential parameters given in Table 5.3.

Moreover, in this case we divided the ANC for $\sqrt{2k}$ in order to have it dimensionless. In Table 5.4 we report the values for $V_0$ and $a_0$, and the calculated values of the binding energies and ANCs for both the GS and FES. Note that, to our knowledge, there are no experimental data for the ANCs.

\[ \eta = 1.439975 \times Z_pZ_{^6\text{Li}} \frac{\mu}{2kh^2}. \]  

(5.17)

\[ \eta = 1.439975 \times Z_pZ_{^6\text{Li}} \frac{\mu}{2kh^2}. \]  

(5.17)
channel. Therefore the $^3$He $\rightarrow$ $^4$He channel results to be hidden in the experimental phase shifts that we reproduce with our potential. On the other hand, for the $^7$Be bound states, the $^3$He $\rightarrow$ $^4$He component has to be considered, and this is done phenomenologically, introducing in our calculation the spectroscopic factors, as explained in the next subsection.

5.3.1 The astrophysical S-factor

The main contribution to the $p + ^6$Li $\rightarrow ^7$Be $+ \gamma$ radiative capture reaction S-factor comes from the electric dipole ($E1$) transition. The structure of the electric operator in the long wavelength approximation implies a series of selection rules due to the presence of the Wigner-6j coefficient as shown in Eq. (5.6). Therefore, the only waves allowed by the $E1$ transition operator up to $L = 2$ are $2S_{1/2}$, $2D_{3/2}$ and $2D_{5/2}$ for the GS, and $2S_{1/2}$ and $2D_{3/2}$ for the FES. From the calculation, it turns out that up to energies of about 400 keV, the contribution of the $^2D$ waves is very small. However, for higher values of the energy, this contribution becomes significant.

In Figure 5.2 we compare our results for the astrophysical S-factor with the experimental data of Ref. [59] and [55]. The calculation is performed summing up the contributions to both the GS and the FES. Since the data of Ref. [59] are still under debate, in discussing the results of Figure 5.2 we will consider only the data of Ref. [55]. By inspection of the figure, we can conclude that our calculated (bare) S-factor is systematically lower than the data. The reason can be simply traced back to the fact that in our model we do not take into account the internal structure of $^6$Li and $^7$Be. In order to overcome this limitation, we introduce the spectroscopic factor $S$, for both bound states of $^7$Be, so that the total cross section can be rewritten as

$$\sigma(E) = S^2_0 \sigma^\text{bare}_0(E) + S^2_1 \sigma^\text{bare}_1(E).$$

(5.18)

Here $\sigma^\text{bare}_0(E)$ and $\sigma^\text{bare}_1(E)$ are the calculated bare cross section and spectroscopic factor for the transition to the GS (FES) of $^7$Be.

In order to determine the two spectroscopic factors $S_0$ and $S_1$, we proceed as follows: we notice that in Ref. [55] there are two sets of data, which corresponds to the radiative capture to GS and FES, and the total S-factor is given by multiplying the data for the relative branching ratio (BR). Therefore, we divide the two data sets for the corresponding BR and we fit the spectroscopic factors, calculating the S-factor for GS and FES captures separately. In such a way we are able to reproduce not only the total S-factor but also the experimental BR for the FES radiative capture of $\sim 39\%$ [55], defined as $S^2_1 \sigma^\text{bare}_1(E)/\sigma(E)$. The values of the spectroscopic factors and the $\chi^2/N$, where $N$ is the number of independent data, are given in Table 5.5. We used the data of Ref. [55] only, before ($\chi^2/N$) and after ($\chi^2/N$) adding the spectroscopic factors.

From the values of the $\chi^2/N$ given in Table 5.5, it is possible to conclude that the description of the radiative capture reaction to the GS using the bare wave function is quite accurate, while this is not the case for the FES.

In order to extrapolate the astrophysical S-factor at zero energy, we perform a polynomial fit of our calculated points up to second order, i.e. we rewrite the S-factor $S(E)$ in the energy range between 0 and 300 keV as

$$S(E) = S(0) + S_1(0)E + S_2(0)E^2.$$  

(5.19)

In Table 5.6 we report the values obtained for $S(0)$, $S_1(0)$, and $S_2(0)$ obtained for our model compared with other phenomenological models of Refs. [61–63].
Chapter 5. The $^6\text{Li} + p \rightarrow ^7\text{Be} + \gamma$ radiative capture reaction

Figu\textit{e 5.2:} Total astrophysical $S$-factor for the $^6\text{Li}(p, \gamma)^7\text{Be}$ radiative capture reaction. The (blue) dashed line is the bare calculation, while the (red) full line is the obtained including the spectroscopic factors $S_0$ and $S_1$ of Table 5.5. The data are taken from Refs. [55] and [59].

| $J^\pi$ | $S$   | $\chi^2_0/N$ | $\chi^2_1/N$ |
|--------|-------|--------------|--------------|
| $3/2^-$ | 1.003 | 0.064        | 0.064        |
| $1/2^-$ | 1.131 | 2.096        | 0.219        |

Table 5.5: Spectroscopic factors $S$ and $\chi^2/N$ obtained by fitting the data of Ref. [55], before ($\chi^2_0/N$) and after ($\chi^2_1/N$) adding the spectroscopic factors themselves. With $J^\pi = 3/2^-$ and $J^\pi = 1/2^-$ we indicate the GS and FES of $^7\text{Be}$.

In particular, we can conclude that all the results for $S(0)$ are within $3\%$. As regarding the shape of the $S$-factor, determined by $S_1(0)$ and $S_2(0)$, our results are quite in agreement with those of Ref. [61] and [63]. On the other hand, the results obtained in Ref. [62] with an approach similar to ours, give a higher value for $S_1(0)$ and $S_2(0)$. The origin of this discrepancy is still unknown. The results of Ref. [64], although obtained with a more sophisticated model than the one presented here, are consistent with ours, while those of Ref. [65] show a different energy dependence. All the theoretical calculations, except the studies of Refs. [57, 58], agree in a negative slope in the $S$-factor at low energies, and none of them predict a resonance structure, as suggested instead by the data of Ref. [59].

In order to estimate the theoretical uncertainty arising from a calculation performed in the phenomenological two-body cluster approach, we have reported in Figure 5.3 in a (gray) band all the results available in literature. As we can conclude by inspection of the figure, the theoretical error which can be estimated by the width of the band is quite significant, of the same order of the experimental errors on the data. If we take into account all the results obtained with the phenomenological potentials of Refs. [61–63] and the results of the present work, we obtain for the
Chapter 5. The $p^6Li \rightarrow ^7Be + \gamma$ radiative capture reaction

Table 5.6: Astrophysical factor at zero energy $S(0)$ and the coefficients $S_1(0)$ and $S_2(0)$ obtained from the polynomial fit of the $S$-factor as defined in Eq. (5.19). For Refs. [61–63] we report the expansion obtained from the fit of digitalized curves of the total $S$-factor.

|                | This work | Ref. [62] | Ref. [61] | Ref. [63] |
|----------------|-----------|-----------|-----------|-----------|
| $S(0)$ [eV b]  | 103.9     | 106       | 98.5      | 108       |
| $S_1(0)$ [eV b/MeV] | $-105.1$ | $-215$    | $-71.5$   | $-130$    |
| $S_2(0)$ [eV b/MeV$^2$] | 45.0      | 312       | 32.5      | 81.7      |

$$S(0) = (103.5 \pm 4.5) \text{ eV b}.$$  \hspace{1cm} (5.20)

We remark that also the value for $S(0)$ obtained in Ref. [101] is within this range.

5.3.2 Angular distribution of photons

We present in this section the photon angular distribution results obtained within the framework outlined in Sec. 5.1, and we compare our results with the data of Ref. [56]. This provides a further check on our model.

By using Eq. (5.12), we have found that the main contribution to the $A_\beta^{13}(E)$ coefficients comes from the interference of the $E1$ multipole generated by the $^2S_{1/2}$ wave with the $E1$ generated by the $^2D$ waves and with the $E2$ generated by the $^2P$ waves. Note that for the $^2P$ and $^2D$ waves, we do not have a complete set of data for the phase shifts for all possible total angular momentum $J^\pi$ values. Therefore we use the same radial function for the $^2D_{3/2}$ and $^2D_{5/2}$ waves, and also for the $^2P_{1/2}$
and $^2P_{3/2}$ waves. The relative phases for these waves, being arbitrary, are fixed in order to have the best description of the data of Ref. [56].

The results for the $A_k^{J_3}$ coefficients for various incident proton energies ($E_p$) are reported in Table 5.7, where they are compared with the values fitted on the experimental data of Ref. [56]. In Figures 5.4 and 5.5 we report the calculated angular distribution of the emitted photon for the capture to the GS and to the FES, respectively, for protons of laboratory energy $E_p = 0.5$ MeV. The data of Ref. [56] are also shown. The theoretical values are in agreement with the fitted data for the GS. In particular, the $A_{3/2}^{3/2}$ coefficient, obtained using Eq. (5.11), results to be

$$A_{3/2}^{3/2} \propto E_1^{121232} \left( E_2^{12232} - E_2^{12322} \right) + \ldots ,$$

where the dots indicate the interferences between the $E1$ generated by the $D$ waves, which give a negligible contribution. If now we suppose that $E_2^{12232} \simeq E_2^{12322}$, the value for $A_{3/2}^{3/2}$ goes to zero, explaining why we do not need this coefficient to reproduce the data. In our case the values of the coefficients $A_{3/2}^{3/2}$ are exactly zero, because we use the same radial function for different $J^\pi$. The same happens also for $A_{3/2}^{1/2}$. As regarding to the capture to the FES, our calculation shows also a nice agreement to the values obtained by fit to the data of Ref. [56]. In this case, there is no cancellation as in Eq. (5.21), and therefore the values of the coefficients $A_k^{1/2}$ are strongly dependent on the $^2P$ and $^2D$ waves, which are very uncertain in our model.

The photon angular distribution has a noticeable impact on the experimental measurements of the $S$-factor. Many experiments are done measuring only the photon emitted in a small part of the total solid angle ($\Omega_d$). Therefore, the rough data must be corrected by a factor related to the angular distribution which enters

| $E_p$ (keV) | $J_3 = 3/2$ | $J_3 = 1/2$ |
|------------|-------------|-------------|
| $k$ | This work | Fit [56] | This work | Fit [56] |
| 1 | 0.000 | - | 0.188 | 0.193 ± 0.055 |
| 2 | 0.210 | 0.299 ± 0.045 | 0.222 | 0.159 ± 0.074 |
| 3 | 0.000 | - | 0.028 | - |
| $\chi^2/N$ | 0.97 | 0.90 | 0.62 | 0.78 |
| $E_p = 800$ keV | | | | |
| 1 | 0.000 | - | 0.237 | 0.283 ± 0.042 |
| 2 | 0.303 | 0.390 ± 0.031 | 0.322 | 0.257 ± 0.051 |
| 3 | 0.000 | - | 0.056 | - |
| $\chi^2/N$ | 0.87 | 1.17 | 1.37 | 0.76 |
| $E_p = 1000$ keV | | | | |
| 1 | 0.000 | - | 0.262 | 0.205 ± 0.043 |
| 2 | 0.354 | 0.368 ± 0.036 | 0.376 | 0.281 ± 0.054 |
| 3 | 0.000 | - | 0.078 | - |
| $\chi^2/N$ | 1.03 | 1.21 | 1.61 | 1.67 |

Table 5.7: Values of the coefficients $A_{3/2}^{3/2}(E)$ and $A_{1/2}^{1/2}(E)$ for three proton energies compared with the fit to the data of Ref. [56]. The $\chi^2/N$ is also reported.
in the determination of the efficiency of the detector. The factor of correction is then given by

\[
\varepsilon(E, \Omega_d) \propto \int_{\Omega_d} d\cos \theta d\phi \left( 1 + \sum_{k \geq 1} A_k(E) P_k(\cos \theta) \right).
\]  

(5.22)

where \(\Omega_d\) is the solid angle of the detector on which the angular distribution is integrated. The LUNA experiment, in order to minimize the effect of the angular distributions, aligned the center of the photon detector to an angle \(\theta_0 \simeq 55^\circ\) respect to the beam axis. In this way the contribution of \(A_{J=1}^{J=3/2}(E)\) is almost negligible since \(P_2(\cos \theta_0) \simeq 0\) and so the integrals between angles close to \(\theta_0\) is quite small. However, the contribution which comes from the \(A_{J=1}^{J=3/2}(E)\) coefficient cannot be neglected. Using our calculations of the coefficient \(A_{J=1}^{J=3/2}(E)\), which are not known experimentally, the LUNA Collaboration was able to estimate the impact of the angular distribution of the photon to the measurement of the \(p + ^6Li \rightarrow ^7Be + \gamma\) cross section. In Figure 5.6 we show the yields, namely the number of photon measured normalized on the number of incoming protons, for the capture to the GS and the FES as function of the incoming proton energy. By inspecting the figure we can conclude that the correction given by the photon angular distribution is negligible for the capture to the GS (less than 0.2%) [103]. This can be traced back to the fact that the coefficient \(A_{J=1}^{1/2}(E) \simeq 0\) and the coefficient \(A_{J=2}^{1/2}(E)\) does not significantly contribute, because of the geometry of the detector. On the other hand, for the FES, the corrections are of the order of \(\sim 6-9\%\) [103], which translates in an appreciable modification of the experimental yield, as can be seen in the figure. As before, this effect is mainly due to the \(A_{J=3}^{3/2}(E)\), coefficient which is not 0 for the FES.

Before concluding the discussion, we want to remark that the poor knowledge on the phase shifts on the \(P\) and \(D\) waves introduce large uncertainties. These were estimated by comparing our angular distributions with the available data and then used in the data analysis performed by the LUNA Collaboration.
Chapter 5. The \( p^+{}^6\text{Li} \rightarrow {}^7\text{Be} + \gamma \) radiative capture reaction

5.3.3 The “He”-resonance

In a recent work [59], He et al. considered the possibility of introducing a resonance-like structure in the \( {}^5\text{Li}(p, \gamma){}^7\text{Be} \) S-factor data at low energies, and they estimated the energy and width in the proton decay channel to be \( E_R = 195 \text{ keV} \) and \( \Gamma_p = 50 \text{ keV} \), respectively. The total angular momentum of the resonance reported in Ref. [59] was conjectured to be either \( J^\pi = 1/2^+ \) or \( J^\pi = 3/2^+ \). In this section we give for granted the existence of this resonance, and we explore the effects of introducing such a resonance structure in our model. The comparison with the available data will tell us whether this assumption is valid or not.

The first step of our study consists in constructing the nuclear potentials in order to obtain \( 190 \text{ keV} < E_R < 200 \text{ keV} \) and to reproduce the width of the resonance in the S-factor data. In a first calculation, we consider to introduce the resonance in the partial wave of spin 1/2. In particular we use the wave \( ^2S_{1/2} \) for \( J^\pi = 1/2^+ \) and \( ^2D_{3/2} \) for \( J^\pi = 3/2^+ \). In both cases, we were not able to find values for the parameters \( V_0 \) and \( a_0 \) [see Eq. (5.13)] that give a consistent description of all the available data. For the \( ^2S_{1/2} \) the introduction of such a resonance is completely inconsistent with the experimental phase shifts. For the \( ^2D_{3/2} \) we do not have experimental constrains on the experimental phase shifts, but we were not able to obtain the strength of the resonance as given in Ref. [59]. The best result obtained adding the resonance in the \( ^2D_{3/2} \) wave is given in Figure 5.7.

In a second calculation, we considered the GS of \( {}^7\text{Be} \) to be a mixed state of spin \( 1/2 \) and \( 3/2 \). In this way the E1 operator can couple the scattering wave \( ^4S_{3/2} \) to the \( ^4P_{3/2} \) component of the GS. Therefore, we can introduce the \( J^\pi = 3/2^+ \) resonance in the \( ^4S_{3/2} \) partial wave. In this calculation, we use the \( ^2P_{3/2} \) radial wave function for the \( ^4P_{3/2} \) component of the GS. We select as potential parameters for the \( ^4S_{3/2} \) component \( V_0 = 438.7 \text{ MeV} \) and \( a_0 = 0.2 \text{ fm}^{-2} \). With this potential we get a resonance energy of \( E_R = 197 \text{ keV} \) and a width of the resonance \( \Gamma \sim 15 \text{ keV} \).

The difference in the width compared to the value reported by Ref. [59] is mainly due to the fact that we do not include interferences with the \( ^3\text{He} - ^4\text{He} \) channel. Then we rewrite the total cross section as

\[
\sigma(E) = S_0^2 \sigma_0^{\text{bare}}(E) + S_1^2 \sigma_1^{\text{bare}}(E) + S_{\text{res}}^2 \sigma_{\text{res}}^{\text{bare}}(E),
\]  

(5.23)
where $S_{\text{res}}$ is the spectroscopic factor of the $^{4}P_{3/2}$ wave component in the GS and $\sigma_{\text{bare}}$ is the calculated capture reaction cross section in the resonance wave. The result obtained imposing $S_{0} = S_{1} \sim 1$ and $S_{\text{res}} \sim 0.011$ is in good agreement with both the data set of Refs. [55] and [59] and it is shown in Figure 5.8. The small value of $S_{\text{res}}$ reflects the small percentage of spin 3/2 component in the $^7\text{Be}$ GS. To be noticed that our results are also consistent with the R-matrix fit reported in Ref. [59]. However, using the potential model which describes the resonance in the $S$-factor data, we were not able to reproduce the $^{4}S_{3/2}$ elastic phase shifts data. Indeed, as shown in Figure 5.9, the $^{4}S_{3/2}$ phase shift is badly underpredicted. Therefore we can conclude that by including the resonance structure in the $^{4}S_{3/2}$ wave, we obtain a nice description of the $S$-factor data, but we destroy the agreement between theory and experiment for the elastic phase shifts. This puts under question the real existence of the resonance structure proposed in Ref. [59].
Chapter 5. The \( p^6\text{Li} \rightarrow ^7\text{Be} + \gamma \) radiative capture reaction

Figure 5.7: Bare astrophysical \( S \)-factor (blue dot-dashed line) to which it is summed a resonance structure in the \( ^2D_{3/2} \) wave (full red line). See text for more details.

Figure 5.8: Bare astrophysical \( S \)-factor (blue dot-dashed line) to which it is summed a resonance structure in the \( ^4S_{3/2} \) wave (full red line). See text for more details.
Chapter 5. The $^6\text{Li} \rightarrow ^7\text{Be} + \gamma$ radiative capture reaction

Figure 5.9: Elastic scattering phase shifts for the $^4S_{3/2}$ wave calculated in the case of resonance (red full line) and no resonance (blue dashed line), compared with the data of Ref. [62].
Chapter 6

Conclusions

In this Thesis we studied two reactions related to the production of $^6$Li in the BBN: the $\alpha + d \to ^6$Li + $\gamma$ and the $p + ^6$Li $\to ^7$Be + $\gamma$ radiative capture reactions.

For the first reaction we used a so-called ab-initio approach, in which we solved the full six-body quantum mechanical problem. In particular, we considered a variational approach, in which we expanded our wave functions in terms of the HH functions. Since solving the full six-body problem is very complex, in this work we moved only the first steps towards the analysis of the $\alpha + d$ radiative capture reaction. In particular, we studied in details the $^6$Li ground state, which is the final state of the reaction. As first we analyzed the convergence rate of the binding energy as function of the number of HH states used in the wave function expansion. In order to reach reasonable convergence, we considered chiral nuclear potentials evolved using the SRG unitary transformation [73], which are usually considered in ab-initio variational approaches. We were able to obtain convergence rates even better than the ones obtained using the NCSM reported in Ref. [74]. On the other hand, in our calculation we did not consider three-body forces which are fundamental to give an accurate description of the nuclear structure. However, in order to have models which give values of the observables close to the experimental one, we have selected SRG transformed interaction for which presumably the effects of proper three-body forces and the ones induced by the SRG evolution cancel out.

Then we focused on $^6$Li electromagnetic static structure. Since we did not considered SRG evolved operators and three-body forces, we were not able to reproduce exactly the experimental values. However, we were able to obtain a lot of information on the $^6$Li structure. In particular, we noticed a strong dependence of the electromagnetic observables on the strength of tensor forces in the nuclear potentials. Moreover, we found indication that two-body electromagnetic currents are presumably needed to explain the small and negative electric quadrupole moment found in the experiments.

Finally, we considered the $\alpha + d$ clusterization of $^6$Li which plays a crucial role in the determination of the astrophysical $S$-factor. Indeed, by defining the overlap between the $^6$Li and the $\alpha + d$ wave functions in relative $S$ and $D$ wave, we were able to obtain the ANCs, which appear squared in the formula for the calculation of the radiative capture cross section. To compute the ANCs we used two different approaches, one computing it directly from the overlap of the wave functions, the other from a differential equation. The results obtained with the two approaches were not compatible within the error bars. However, we considered the second approach more reliable, since in the first one there are systematic uncertainties which cannot be properly controlled. The obtained values well reproduce the correct magnitude of the experimental values of the ANCs. The result is quite remarkable, if we consider that the potential models we used have no parameters constrained on this particular nuclear system.
The most important result of this work is the extension of the HH approach to nuclei up to $A = 6$ mass number. In the Thesis we have presented not only the theoretical aspect but also some of the algorithmic improvements needed to perform calculations at $A = 6$. In perspective, using more refined computing codes, we believe possible to increase the HH basis compared to the one used in this work. Therefore we expect that it will be possible for the first time with an *ab-initio* variational approach to reach good convergence with not-SRG evolved potentials at $A = 6$. Moreover, in this work we established the first steps towards the *ab-initio* study calculation of the $\alpha + d$ scattering. In solving scattering problems, the main difficulty is to compute the potential matrix elements between scattering states and pure HH states. In this work, we presented and validated an approach that permits to project scattering states on the HH basis making easy then to compute the potential matrix elements. Therefore, this Thesis can be considered as the starting point of the application of the HH approach to study a wide range of nuclear phenomena that appear at $A = 6$.

To study of the $p + ^6\text{Li} \rightarrow ^7\text{Be} + \gamma$ we used a phenomenological approach in which we treated $p$ and $^6\text{Li}$ as structureless particles. In this approach the parameters of the phenomenological nuclear potential are fitted in order to reproduce the experimental binding energies and scattering phase shifts. The theoretical $S$-factor is able to reproduce the experimental data once we introduced the spectroscopic factor to take care of the internal structure of the colliding nuclei. By comparing different phenomenological approaches presented in the literature, we estimated also a theoretical error for the $S$-factor.

The main goal of this study was the determination of the photon angular distribution, which is an unknown input for determining the efficiency of experimental setups. We validated our theoretical calculations obtained with our model by comparing with the available data. Then, they were used to determine the efficiency of the LUNA experimental setup and determine the final experimental yields.

Finally, we have studied the possibility of introducing in our model the resonance-like structure proposed in Ref. [59]. Even if, by introducing it in the $^4S_{3/2}$ partial wave, we were able to obtain a nice description of the $S$-factor data as given in Ref. [59], we completely lost the possibility to reproduce the $^4S_{3/2}$ experimental scattering phase shifts. We can conclude therefore that the presence of a resonant structure cannot be accepted in our theoretical framework.
Appendix A

The Transformation Coefficients

In this appendix we present the calculation of the TC as defined in Eq. (2.55). We follow the method presented in Refs. [104, 105], based on the recursion relations, generalizing the formulas for the $A=6$ case. This appendix is divided in three sections. In Section A.1 we introduce the various terms needed to construct the TC. In Section A.2 we discuss the recursion procedure. Finally in Section A.3 we present the orthogonalization procedure.

A.1 Construction of the Transformation Coefficients

The TC are defined in Chapter 2 as the coefficients $a_{\alpha,\alpha'}^{KLSTJ\pi}(p)$ which transforms a state $\alpha$, written in a generic permutation $p$, in a sum of states $\alpha'$ written in the reference permutation, namely

$$\Phi^{|KLSTJ\pi\alpha\rangle}_{\alpha}(i,j,k,l,m,n) = \sum_{\alpha'} a_{\alpha,\alpha'}^{KLSTJ\pi}(p)\Phi^{|KLSTJ\pi\alpha'\rangle}_{\alpha'}(1,2,3,4,5,6),$$  \hspace{1cm} (A.1)

where $\alpha$ is defined in Eq. (2.50) and $\Phi^{|KLSTJ\pi\rangle}_{\alpha}(i,j,k,l,m,n)$ is defined in Eq. (2.49). By construction, the functions $\Phi^{|KLSTJ\pi\rangle}_{\alpha}(i,j,k,l,m,n)$ are the product of a HH, a spin and an isospin function. We can define coefficients that transform each part from a permutation to another. Therefore, for the HH part we define the coefficients $c_{KL,p}^{\mu,\mu'}$ such that

$$Y^{|KL,p\rangle}_{\mu} = \sum_{\mu'} c_{KL,p}^{\mu,\mu'} Y^{|KLM,1\rangle}_{\mu'},$$ \hspace{1cm} (A.2)

where $Y^{|KLM,p\rangle}_{\mu}$ is defined in Eq. (2.44) and the apex $p$ indicates that the HH function depends on $\Omega_{5p}$. We will discuss the calculation of this coefficients in Section A.2.

As regarding the spin(isospin) part, we define similar coefficients $c_{S,T}^{\sigma,\sigma'}(c_{S,S}^{\tau,\tau'})$, such that

$$S_{\sigma}^{|SSz,p\rangle} = \sum_{\sigma'} c_{\sigma,\sigma'}^{S,p} S_{\sigma'}^{|SSz,1\rangle},$$ \hspace{1cm} (A.3)

where $\sigma = \{S_2, S_3, S_4, S_5, S\}$, and

$$S_{\sigma}^{|SSz,p\rangle} = \left[ (s_i s_j)_{S_2} s_k \right]_{S_3} \left[ (s_l s_m)_{S_4} s_n \right]_{S_5},$$ \hspace{1cm} (A.4)

and analogously for the isospin. By using Eq. (A.3) it is possible to compute the coefficients as

$$c_{\sigma,\sigma'}^{S,p} = \left( S_{\sigma}^{|SSz,1\rangle} \right)_{\tau} S_{\sigma}^{|SSz,p\rangle},$$ \hspace{1cm} (A.5)
which can be written explicitly as a sum of products of Clebsch-Gordan coefficients
that, for the specific used coupling scheme, reads
\[
\hat{c}_{\sigma'\sigma}^{S,p} = \sum_{m_1,m_2,m_3} \sum_{m_4,m_5,m_6} (S_3 M_3, S_5 M_5 | S M_6)(S_3' M_3', S_5' M_5' | S M_6)
\times (S_2 M_2, \frac{1}{2} m_3|S_3 M_3)(S_4 M_4, \frac{1}{2} m_6|S_5 M_5)(S_4' M_4', \frac{1}{2} m_6|S_5' M_5')
\times (\frac{1}{2} m_1, \frac{1}{2} m_2|S_2 M_2)(\frac{1}{2} m_4, \frac{1}{2} m_5|S_4 M_4)(\frac{1}{2} m_1, \frac{1}{2} m_m|S_4' M_4'),
\]
where \(M_i = m_i + M_{i-1}\) with \(M_0 = 0\). This formula is valid also for the isospin part, substituting \(S, \sigma\) and \(\sigma'\) with \(T, \tau\) and \(\tau'\), respectively. By definition, a state \(\alpha\) in a generic permutation \(p\) can be written as
\[
\Phi^{KLSTJ_{\pi}}_{\alpha}(i, j, k, l, m, n) = [\gamma_{\mu}^{KL,p} S_{\sigma'}^{SS_{\pi},p}]_{J\tau} \tau'_{T,T},
\]
where, by definition, \(\alpha = \{\mu, \sigma, \tau\}\). Using Eqs. (A.2) and (A.3), Eq. (A.7) reads
\[
\Phi^{KLSTJ_{\pi}}_{\alpha}(i, j, k, l, m, n) = \sum_{\mu'} \sum_{\sigma'} \sum_{\tau'} [c_{\mu'\mu', \sigma'\sigma, \tau'\tau}^{KL,p}] [\gamma_{\mu'}^{KLM,1} S_{\sigma'}^{SS_{\pi},1}]_{J\tau} \tau'_{T,T}.\]
Comparing Eq. (A.1) with Eq. (A.8), it is easy to derive the final expression for the TC in terms of the coefficients \(c\), i.e.
\[
a^{KLSTJ_{\pi}}_{\alpha,\alpha'}(p) = [c_{\mu'\mu, \sigma'\sigma, \tau'\tau}^{KL,p}]_{T,P}.\]

Once constructed the TC for each permutation, we can evaluate the coefficients \(A^{KLSTJ_{\pi}}_{\alpha,\alpha'}\) as given in Eq. (2.57).

### A.2 The recursion procedure

In this section we discuss the calculation of the coefficients \(c_{\mu'\mu, \sigma'\sigma, \tau'\tau}^{KL,p}\). In order to make the notation easier we rewrite the generic HH function, defined in Eq. (2.44), as
\[
\gamma_{\mu}^{KLM}(\Omega_{5p}) = \left[\left((Y_{\ell_1}(\hat{x}_1 p)Y_{\ell_2}(\hat{x}_2 p))_{L_2} Y_{\ell_3}(\hat{x}_3 p)\right)_{L_3} Y_{\ell_4}(\hat{x}_4 p)\right]_{L_4} Y_{\ell_5}(\hat{x}_5 p),
\]
where
\[
y_{jp} = \cos 2\varphi_{jp},
\]
and the hyperangles \(\varphi_{jp}\) are defined in Eq. (2.7). The \(P_{\nu_j}^{\ell_j-\ell_j+1/2}(y_{jp})\) are the Jacobi polynomials, and
\[
N_{\nu_j,K_{j-1}}^{\ell_j,\nu_j} = \left(\frac{1}{2}\right)\left(\frac{L_j+K_{j-1}}{2}\right) \left[\frac{2\nu_j\Gamma(\nu_j-n_j)n_j!}{\Gamma(\nu_j-n_j-\ell_j-1/2)\Gamma(n_j+\ell_j+3/2)}\right]^{1/2},
\]
are normalization factors [see Eq. (2.33)], where \(\nu_j\) and \(K_j\) are defined in Eq. (2.28). The index \(\mu\) in Eq. (A.10) has been introduced in Eq. (2.46).
Appendix A. The Transformation Coefficients

Let us assume to know the coefficients \( c_{\mu \mu'}^{KLM} \) for a given \( K \), so that

\[
\mathcal{Y}_{\lambda, n_2, n_3, n_4, n_5}^{KLM} = \sum_{\mu'} c_{\lambda, n_2, n_3, n_4, n_5; \mu; \mu'}^{KLM} \mathcal{Y}_{\mu, 1}^{KLM},
\]

(\ref{eq:coefficients})

where for convenience, we have defined

\[
\lambda = \{ \ell_1, \ell_2, \ell_3, \ell_4, \ell_5, L_2, L_3, L_4 \}.
\]

(\ref{eq:quantum_numbers})

The recurrence is applied separately on the quantum number \( n_2, n_3, n_4 \) and \( n_5 \), once fixed the quantum numbers \( \lambda \).

In the following we will use the quantities

\[
a_{n_i} = \frac{N^{\ell_1, \ldots, \ell_5}_{n_2, \ldots, n_i + 1, 0, \ldots, 0}}{N^{\ell_1, \ldots, \ell_5}_{n_2, \ldots, n_i, 0, \ldots, 0}} \left( \frac{(2n_i + \alpha_i + \beta_i + 1)(\alpha_i^2 - \beta_i^2)}{2(n_i + 1)(n_i + \alpha_i + \beta_i + 1)(2n_i + \alpha_i + \beta_i)} \right),
\]

(\ref{eq:an_i})

\[
b_{n_i} = \frac{N^{\ell_1, \ldots, \ell_5}_{n_2, \ldots, n_i + 1, 0, \ldots, 0}}{N^{\ell_1, \ldots, \ell_5}_{n_2, \ldots, n_i, 0, \ldots, 0}} \left( \frac{(2n_i + \alpha_i + \beta_i + 1)(2n_i + \alpha_i + \beta_i + 2)}{(n_i + 1)(n_i + \alpha_i + \beta_i + 1)} \right),
\]

(\ref{eq:bn_i})

\[
c_{n_i} = -\frac{N^{\ell_1, \ldots, \ell_5}_{n_2, \ldots, n_i + 1, 0, \ldots, 0}}{N^{\ell_1, \ldots, \ell_5}_{n_2, \ldots, n_i, 0, \ldots, 0}} \left( \frac{(n_i + \alpha_i)(n_i + \beta_i)(2n_i + \alpha_i + \beta_i + 2)}{(n_i + 1)(n_i + \alpha_i + \beta_i + 1)(2n_i + \alpha_i + \beta_i)} \right),
\]

(\ref{eq:cn_i})

which are defined for \( i = 2, \ldots, 5 \). Here we have defined \( \alpha_i = \nu_{i-1}, \beta_i = \ell_i + 1/2 \) and

\[
N^{\ell_1, \ldots, \ell_N}_{n_1, \ldots, n_5} = \prod_{j=2}^{5} N^{\ell_j, \nu_j}_{n_j, K_j-1}.
\]

(\ref{eq:relations})

If we consider the function \( \mathcal{Y}_{\lambda, n_2, n_3, n_4, n_5 + 1}^{KLM} \), the Jacobi polynomial \( P_{n_5 + 1}(y_{5p}) \) entering the expression can be written in terms of \( P_{n_5}(y_{5p}) \) and \( P_{n_5 - 1}(y_{5p}) \) by using the Jacobi polynomial recursion relation. Explicitly we obtain

\[
\mathcal{Y}_{\lambda, n_2, n_3, n_4, n_5 + 1}^{KLM} = (a_{n_5} + b_{n_5} y_{5p}) \mathcal{Y}_{\lambda, n_2, n_3, n_4, n_5}^{KLM} + c_{n_5} \mathcal{Y}_{\lambda, n_2, n_3, n_4, n_5 - 1}^{KLM}.
\]

(\ref{eq:coefficients2})

Now, \( y_{5p} = 2 \left( \frac{x_{5p}}{\rho} \right)^2 - 1 \), and

\[
\left( \frac{x_{lp}}{\rho} \right)^2 = \sum_{i,j} \Gamma_{i,j}^l \mathbf{x}_i \cdot \mathbf{x}_j \quad l, i, j = 1, \ldots, 5,
\]

(\ref{eq:jacobi_vectors})

\( \mathbf{x}_i \) being the Jacobi vectors evaluated in the permutation 1 and in this case \( l = 5 \). The coefficients \( \Gamma_{i,j}^l \) are numerical coefficients which depend on the permutation. Using the orthonormalization properties of the HH functions, one gets

\[
c_{\mu \mu'}^{K+2LM} = \int d\Omega \left[ \mathcal{Y}_{\mu}^{K+2LM} (\Omega_5) \right]^{\dagger} \mathcal{Y}_{\mu'}^{K+2LM} (\Omega_{5p}),
\]

(\ref{eq:coefficients3})

where

\[
\int d\Omega_5 = \frac{1}{2^5} \int_{i=1}^{5} d\hat{x}_i \prod_{j=2}^{5} dy_j (1 + y_j)^{\frac{1}{2}} (1 - y_j)^{\frac{-5}{2}}.
\]

(\ref{eq:factorial})

If now we insert Eq. (\ref{eq:coefficients2}) in the integral (\ref{eq:coefficients3}), only the term containing the factor \( b_{n_5} (x_{5p})^2 \) gives a non-vanishing contribution. Indeed only this term is of order \( K + 2 \).
in Eq. (A.19). Finally, by using Eq. (A.13), the recursion relation is obtained
\[ c^{K+2L,p}_{\lambda, n_2, n_3, n_4, n_5, 1; \mu} = 2b_{n_3} \sum_{\mu''} c^{KL,p}_{\lambda, n_2, n_3, n_4, n_5; \mu''} \times \sum_{i,j} I_{i,j}^p(5) I_{i,j}^{\mu''}, \] (A.23)

where
\[ I_{i,j}^{\mu''} = \int d\Omega_5 \left[ \frac{\gamma^{K+2LM}(\Omega_5)}{\rho^2} \right] \Psi^{KL,p}(\Omega_5). \] (A.24)

The explicit expressions for the integrals \( I_{i,j}^{\mu''} \) for \( A = 6 \) are given in Section A.2.1.

Let us now consider the HH function \( \gamma^{KL,p}_{\lambda, n_2, n_3, n_4, n_5, 1} \). By proceeding as in the previous case we have
\[ \gamma^{K+2LM,p}_{\lambda, n_2, n_3, n_4, n_5, 1, 0} = (1 - y_5p)(a_{n_4} + b_{n_4}y_4p)\gamma^{KL,p}_{\lambda, n_2, n_3, n_4, 0} + c_{n_4}(1 - y_5p)^2 \gamma^{K-2LM,p}_{\lambda, n_2, n_3, n_4, 1, 0}. \] (A.25)

The first term of Eq. (A.25) can be written as
\[ (1 - y_5p)(a_{n_4} + b_{n_4}y_4p)\gamma^{KL,p}_{\lambda, n_2, n_3, n_4, 0} = \left[ 4b_{n_4} \frac{(x_4p)^2}{\rho^2} + 2(b_{n_4} - a_{n_4}) \frac{(x_5p)^2}{\rho^2} \right] \gamma^{KL,p}_{\lambda, n_2, n_3, n_4, 0} + \mathcal{O}(K), \] (A.26)

where with \( \mathcal{O}(K) \) we group all the terms of order smaller than \( K + 2 \), which, therefore, do not contribute to the integral in Eq. (A.21). The square of the moduli of the Jacobi vectors \( (x_5p)^2 \) and \( (x_4p)^2 \) can be expressed using Eq. (A.20). The second term in Eq. (A.25) can be rewritten as
\[ (1 - y_5p)^2 \gamma^{K-2LM,p}_{\lambda, n_2, n_3, n_4, 1, 0} = A^{(4)}_{n_2, n_3, n_4, n_5, 1} \gamma^{KL,p}_{\lambda, n_2, n_3, n_4, 0} + B^{(4)}_{n_2, n_3, n_4, n_5, 1} \gamma^{KL,p}_{\lambda, n_2, n_3, n_4, 0} + C^{(4)}_{n_2, n_3, n_4, n_5, 1} \gamma^{KL,p}_{\lambda, n_2, n_3, n_4, 0}, \] (A.27)

where we expressed the factor \( (1 - y_5p)^2 \) in terms of the Jacobi polynomials of order 0, 1 and 2. Above, we have defined
\[ A^{(i)}_{n_2, n_3, n_4} = \frac{N_{n_2, n_3, n_4, 0, 0}}{N_{n_2, n_3, n_4, 0, 0}} \left( \frac{8}{(\alpha_i + \beta_i + 4)(\alpha_i + \beta_i + 3)} \right), \] (A.28)
\[ B^{(i)}_{n_2, n_3, n_4} = \frac{N_{n_2, n_3, n_4, 0, 0}}{N_{n_2, n_3, n_4, 0, 0}} \left( \frac{8(\alpha_i + 2)}{(\alpha_i + \beta_i + 4)(\alpha_i + \beta_i + 3)} \right), \] (A.29)
\[ C^{(i)}_{n_2, n_3, n_4} = \frac{(\alpha_i + 2)(\alpha_i + \beta_i + 3)(\alpha_i + \beta_i + 2)}{(\alpha_i + \beta_i + 3)(\alpha_i + \beta_i + 2)}, \] (A.30)

where \( \alpha_i = \beta_{i-1} \) and \( \beta_i = \ell_i + 1/2 \). When the expression in Eq. (A.27) is inserted in Eq. (A.21), only the term proportional to \( A^{(4)}_{n_2, n_3, n_4, n_5, 1} \) survives, having order \( K + 2 \).

In conclusion, writing the integral with respect to \( \Omega_5 \) in terms of the integral \( I_{i,j}^{\mu''} \), the recursion formula for \( n_4 \) results
\[ c^{K+2L,p}_{\lambda, n_2, n_3, n_4, n_5, 1; \mu} = c_{n_4} A^{(4)}_{n_2, n_3, n_4, n_5, 1} \gamma^{KL,p}_{\lambda, n_2, n_3, n_4, 0, 0} + \sum_{\mu''} c^{KL,p}_{\lambda, n_2, n_3, n_4, 0; \mu''} \times \sum_{i,j} \left[ 4b_{n_4} I_{i,j}^p(4) + 2(b_{n_4} - a_{n_4}) I_{i,j}^p(5) \right] I_{i,j}^{\mu''}. \] (A.31)
In the case of the HH function $\mathcal{Y}_{\lambda,n_2,n_3+1,0,0}^{K,L,M,p}$, using the recursion of the Jacobi polynomials on the index $n_3$ we get

\begin{equation}
\mathcal{Y}_{\lambda,n_2,n_3+1,0,0}^{K+2L,M,p} = (1 - y_5p)(1 - y_4p)(a_{n_3} + b_{n_3}y_2p)\mathcal{Y}_{\lambda,n_2,n_3,0,0}^{KLM,p} + c_{n_3} (1 - y_5p)^2 (1 - y_4p)^2 \mathcal{Y}_{\lambda,n_2,n_3-1,0,0}^{K-2L,M,p}, \tag{A.32}
\end{equation}

The first term of Eq. (A.32) can be written as

\begin{equation}
(1 - y_5p)(1 - y_4p)(a_{n_3} + b_{n_3}y_2p)\mathcal{Y}_{\lambda,n_2,n_3,0,0}^{KLM,p} = \left[ 8b_{n_3} \frac{(x_3y_2p)^2}{\rho^2} + 4(b_{n_3} - a_{n_3}) \left( \frac{(x_4p)^2}{\rho^2} + \frac{(x_5p)^2}{\rho^2} \right) \right] \mathcal{Y}_{\lambda,n_2,n_3,0,0}^{KLM,p} + \mathcal{O}(K), \tag{A.33}
\end{equation}

where the terms $\mathcal{O}(K)$ do not give contributions when inserted in Eq. (A.21). The second term of Eq. (A.32) is rewritten as

\begin{equation}
(1 - y_5p)^2 (1 - y_4p)^2 \mathcal{Y}_{\lambda,n_2,n_3-1,0,0}^{K-2L,M,p} = A_{n_2,n_3-1}^{(3)} \mathcal{Y}_{\lambda,n_2,n_3-1,0,0}^{K+2L,M,p} + B_{n_2,n_3-1}^{(4)} Y_{\lambda,n_2,n_3-1,1,1}^{K+2L,M,p} + C_{n_2,n_3-1}^{(3)} A_{n_2,n_3-1}^{(4)} Y_{\lambda,n_2,n_3-1,0,0}^{K+2L,M,p} + \mathcal{O}(K), \tag{A.34}
\end{equation}

where we define

\begin{equation}
\eta_{n_2,...,n_i}^{(i)} = \frac{N_{l_1,...,l_5}^{n_2,...,n_i,0,0,...,0}}{(\alpha_i + \beta_i + 2!)}, \tag{A.35}
\end{equation}

\begin{equation}
\gamma_{n_2,...,n_i}^{(i)} = \frac{2(\alpha_i + 1)}{(\alpha_i + \beta_i + 2)!}, \tag{A.36}
\end{equation}

with $\alpha_i = \nu_i$ and $\beta_i = \ell_{i+1} + 1/2$. Inserting these results in Eq. (A.21), we obtain the recursion formula for $n_3$, which reads

\begin{equation}
c_{n_2,n_3+1,0,0,\mu'}^{K+2L,M,p} = c_{n_3} \left[ A_{n_2,n_3-1}^{(3)} c_{n_2,n_3-1,0,\mu'}, A_{n_2,n_3-1}^{(4)} c_{n_2,n_3-1,0,0,\mu'}, c_{n_2,n_3-1}^{(3)} A_{n_2,n_3-1}^{(4)} K+2L,M,p \right] + \sum_{\nu''} c_{n_2,n_3,0,0,\mu''}^{K,L,M,p} \times \sum_{i,j} \left[ 8b_{n_3} \Gamma_{i,j}^p (3) + 4(b_{n_3} - a_{n_3})(\Gamma_{i,j}^p (4) + \Gamma_{i,j}^p (5)) \right] \Gamma_{i,j}^{\mu',\mu''}. \tag{A.37}
\end{equation}

The last recursion is done on the index $n_2$. Imposing $n_3, n_4, n_5 = 0$, we rewrite the HH function $\mathcal{Y}_{\lambda,n_2+1,0,0,0}^{K+2L,M,p}$ using the recursion relation on the Jacobi polynomials, i.e.

\begin{equation}
\mathcal{Y}_{\lambda,n_2+1,0,0,0}^{K+2L,M,p} = (1 - y_5p)(1 - y_4p)(a_{n_2} + b_{n_2}y_2p)\mathcal{Y}_{\lambda,n_2,0,0,0}^{KLM,p} + c_{n_2} (1 - y_5p)^2 (1 - y_4p)^2 (1 - y_3p)^2 \mathcal{Y}_{\lambda,n_2-1,0,0,0}^{K-2L,M,p}, \tag{A.38}
\end{equation}

The first term of Eq. (A.38) can be expressed as

\begin{equation}
(1 - y_5p)(1 - y_4p)(a_{n_2} + b_{n_2}y_2p)\mathcal{Y}_{\lambda,n_2,0,0,0}^{KLM,p} = \left[ 8b_{n_2} \frac{(x_3y_2p)^2}{\rho^2} - \frac{(x_3y_2p)^2}{\rho^2} \right] + 8a_{n_2} \left[ \frac{(x_4p)^2}{\rho^2} + \frac{(x_5p)^2}{\rho^2} \right] \mathcal{Y}_{\lambda,n_2,0,0,0}^{KLM,p} + \mathcal{O}(K), \tag{A.39}
\end{equation}

where also in this case the $\mathcal{O}(K)$ terms do not give contributions in the integrals of...
Eq. (A.21). We can rewrite the factor \((1 - y_{5p})^2(1 - y_{4p})^2(1 - y_{3p})^2\) of the first term in Eq. (A.38) using the Jacobi polynomial of order 0, 1, and 2. Here we report the final result, which reads

\[
(1 - y_{5p})^2(1 - y_{4p})^2(1 - y_{3p})^2 \mathcal{V}^{K-2LM,p}_{n_2,n_2-1,0,0} = A^{(2)}_{n_2-1} \mathcal{V}^{K+2LM,p}_{n_2,n_2-1,2,0,0} + B^{(2)}_{n_2-1} \left[ \eta^{(3)}_{n_2-1,1} \mathcal{V}^{K+2LM,p}_{n_2,n_2-1,1,1,0} + \gamma^{(3)}_{n_2-1,1} \eta^{(4)}_{n_2-1,1,0} \mathcal{V}^{K+2LM,p}_{n_2,n_2-1,1,0,1} \right] + C^{(2)}_{n_2-1} \left[ A^{(3)}_{n_2,0} \mathcal{V}^{K+2LM,p}_{n_2,n_2-1,0,2,0} + B^{(3)}_{n_2-1,0} \eta^{(4)}_{n_2-1,0,1} \mathcal{V}^{K+2LM,p}_{n_2,n_2-1,0,1,1} \right] + C^{(3)}_{n_2-1,0} A^{(4)}_{n_2-1,0,0,0,2} + \mathcal{O}(K),
\]

(A.40)

where again the terms \(\mathcal{O}(K)\) can be discarded in Eq. (A.21). Inserting these result in Eq. (A.21) we get the final expression for the recursion on \(n_2\)

\[
c^{K+2L,p}_{\lambda,n_2+1,0,0,0,0} = c_{n_2} \left[ A^{(2)}_{n_2-1} c^{K+2L,p}_{\lambda,n_2,2,0,0,0,0} + B^{(2)}_{n_2-1} \left( \eta^{(3)}_{n_2-1,1} c^{K+2L,p}_{\lambda,n_2-1,1,1,0,0,0} + \gamma^{(3)}_{n_2-1,1} \eta^{(4)}_{n_2-1,1,0} c^{K+2L,p}_{\lambda,n_2-1,1,0,1,0,0,0} \right) + C^{(2)}_{n_2-1} \left[ A^{(3)}_{n_2-1,0,0} c^{K+2L,p}_{\lambda,n_2-1,0,2,0,0,0} + B^{(3)}_{n_2-1,0,0} \eta^{(4)}_{n_2-1,0,1} c^{K+2L,p}_{\lambda,n_2-1,0,1,1,0,0,0} + C^{(3)}_{n_2-1,0,0} A^{(4)}_{n_2-1,0,0,0} c^{K+2L,p}_{\lambda,n_2-1,0,0,0,2,0,0,0} \right] \right] + \sum_{\mu''} c^{K+2L,p}_{\lambda,n_2,0,0,0,0,\mu''} \sum_{\mu,\nu} \left[ 8 \langle b_{n_2} + a_{n_2} \rangle \Gamma_{\mu,\nu}^{p} \langle 2 \rangle + 8 \langle b_{n_2} - a_{n_2} \rangle \Gamma_{\mu,\nu}^{p} \langle 1 \rangle \right] \langle \mu,\nu \rangle^{p,\mu''}.
\]

(A.41)

Eqs. (A.23), (A.31), (A.37) and (A.41) are the recurrence relations giving the coefficients at order \(K + 2\) in terms of grandangular momentum quantum number \(K\). It is possible to notice that writing the recursion in this way there are no inconsistency. Indeed, the coefficients \(c^{K+2L,p}_{\lambda,n_2,n_3,n_4,n_5+1,0\mu''}\) depend only on the coefficients with grandangular momentum \(K\). The coefficients \(c^{K+2L,p}_{\lambda,n_2,n_3,n_4+1,0,0,\mu''}\) depend on the coefficients at order \(K\) and only on the order \(K + 2\) coefficients evaluated in the recursion on \(n_5+1\), and so on for all the other recursions. Moreover, the four relations already involve only coefficients with the same quantum numbers \(\lambda\). Therefore, the algorithm is well suited in our case, since we need to compute TC up to different \(K\) for different values of \(\lambda\).

In order to complete the discussion we compute the starting case of the recursion by using an approach similar to the one presented in Ref. [106]. Fixed \(L\) and the minimum valid value of \(K\) for this \(L\), we generate \(N\) sets of Jacobi coordinates in a random way, where \(N\) is the number of states \(\mu\) allowed by \(K\) and \(L\). For any choice \(j\) of the Jacobi coordinates, the following relation must be verified

\[
\sum_{\mu'} c^{K,p}_{\mu,\mu'} \gamma^{KLM}_{\mu} \langle \Omega_5(j) \rangle = \gamma^{KLM}_{\mu} \langle \Omega_{5p}(j) \rangle,
\]

(A.42)

where the \(c^{K,L,p}_{\mu,\mu'}\) coefficients are unknown. If we consider the \(N\) sets of Jacobi coordinates, we have \(N\) independent equations for \(N\) unknowns which can be solved with standard algebraic techniques. In principle, this method can be used to find the transition coefficients at any order \(K\), but the numerical precision of the calculation decrease rapidly as the order \(K\) increases. We have used this method to compute the starting TC corresponding to \(n_2 = n_3 = n_4 = n_5 = 0\) so \(K = \ell_1 + \ell_2 + \ell_3 + \ell_4 + \ell_5\). Since this value is always small, the number \(N\) of HH functions is not critical. Moreover, we used this approach for selected cases of \(K > \ell_1 + \ell_2 + \ell_3 + \ell_4 + \ell_5\) as benchmark for the recursion method in order to test the previous formulas and to debug the code.
Appendix A. The Transformation Coefficients

A.2.1 The integrals $I_{i,j}^{\mu,\mu'}$

In this section, we present the detailed calculation for the integrals $I_{i,j}^{\mu,\mu'}$ defined in Eq. (A.24). The integrals $I_{i,j}^{\mu,\mu'}$ involve only functions constructed with the Jacobi polynomials in the permutation $p = 1$. In the case $A = 6$, there are 15 different terms $(\mathbf{x}_i \cdot \mathbf{x}_j)/\rho^2$, which have the following expression in terms of the hyperangular variables $\Omega_5 \equiv \{\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{x}_4, \hat{x}_5, y_2, y_3, y_4, y_5\}$:

\[
\begin{align*}
  x_1^2 \rho^2 & = \frac{(1 - y_5)(1 - y_4)(1 - y_3)(1 - y_2)}{16}, \\
  x_1 \cdot x_2 \rho^2 & = -\frac{4\pi (1 - y_5)(1 - y_4)(1 - y_3)\sqrt{(1 - y_2^2)}}{\sqrt{3}} [Y_1(\hat{x}_1)Y_1(\hat{x}_2)]_{00}, \\
  x_1 \cdot x_3 \rho^2 & = -\frac{4\pi (1 - y_5)(1 - y_4)\sqrt{(1 - y_3^2)(1 - y_2)}}{\sqrt{3}} [Y_1(\hat{x}_1)Y_1(\hat{x}_3)]_{00}, \\
  x_1 \cdot x_4 \rho^2 & = -\frac{4\pi (1 - y_5)\sqrt{(1 - y_4^2)(1 - y_3)(1 - y_2)}}{\sqrt{3}} [Y_1(\hat{x}_1)Y_1(\hat{x}_4)]_{00}, \\
  x_1 \cdot x_5 \rho^2 & = -\frac{4\pi \sqrt{(1 - y_5^2)(1 - y_4)(1 - y_3)(1 - y_2)}}{\sqrt{3}} [Y_1(\hat{x}_1)Y_1(\hat{x}_5)]_{00}, \\
  x_2^2 \rho^2 & = \frac{(1 - y_5)(1 - y_4)(1 - y_3)(1 + y_2)}{16}, \\
  x_2 \cdot x_3 \rho^2 & = -\frac{4\pi (1 - y_5)(1 - y_4)\sqrt{(1 - y_3^2)(1 + y_2)}}{\sqrt{3}} [Y_1(\hat{x}_2)Y_1(\hat{x}_3)]_{00}, \\
  x_2 \cdot x_4 \rho^2 & = -\frac{4\pi (1 - y_5)\sqrt{(1 - y_4^2)(1 - y_3)(1 + y_2)}}{\sqrt{3}} [Y_1(\hat{x}_2)Y_1(\hat{x}_4)]_{00}, \\
  x_2 \cdot x_5 \rho^2 & = -\frac{4\pi \sqrt{(1 - y_5^2)(1 - y_4)(1 - y_3)(1 + y_2)}}{\sqrt{3}} [Y_1(\hat{x}_2)Y_1(\hat{x}_5)]_{00}, \\
  x_3^2 \rho^2 & = \frac{(1 - y_5)(1 - y_4)(1 + y_3)}{8}, \\
  x_3 \cdot x_4 \rho^2 & = -\frac{4\pi (1 - y_5)\sqrt{(1 - y_4^2)(1 + y_3)}}{\sqrt{3}} [Y_1(\hat{x}_3)Y_1(\hat{x}_4)]_{00}, \\
  x_3 \cdot x_5 \rho^2 & = -\frac{4\pi \sqrt{(1 - y_5^2)(1 - y_4)(1 + y_3)}}{\sqrt{3}} [Y_1(\hat{x}_3)Y_1(\hat{x}_5)]_{00}, \\
  x_4^2 \rho^2 & = \frac{(1 - y_5)(1 + y_4)}{4}, \\
  x_4 \cdot x_5 \rho^2 & = -\frac{4\pi \sqrt{(1 - y_5^2)(1 + y_4)}}{\sqrt{3}} [Y_1(\hat{x}_4)Y_1(\hat{x}_5)]_{00}, \\
  x_5^2 \rho^2 & = \frac{(1 + y_5)}{2}.
\end{align*}
\]

By using these relations the integrals of Eq. (A.24) can be factorized in products of five integrals of the kind

\[
\mathcal{J}_j \left[ \ell'_j, m'_j, \ell, m, \ell''_j, m''_j \right] = \int d\hat{x}_j \left[ Y_{\ell'_j m'_j}(\hat{x}_j) \right]^* Y_{\ell m}(\hat{x}_j) Y_{\ell''_j m''_j}(\hat{x}_j),
\]

(A.58)
Appendix A. The Transformation Coefficients

where $j$ goes from 1 to 5 and $\ell = 0$ or 1, and four integrals of the kind

$$I_j(2a, 2b) = \int_{-1}^{1} dy_j (1 - y_j)^a(1 + y_j)^b P_{n_j}^{\nu_j, \delta_j + \frac{3}{2}}(y_j), \quad (A.59)$$

where $j$ goes from 2 to 5.

The integrals type $I_j$ can be easily calculated in terms of Wigner 3j coefficients. The integrals $I_j$ can be evaluated by using Gauss integration formula. Let us define the polynomial

$$P_N(x) = (1 - x)^{\text{int}(a)}(1 + x)^{\text{int}(b)} P_n^{\nu, \ell + \frac{3}{2}}(x) P_n^{\nu', \ell' + \frac{3}{2}}(x), \quad (A.60)$$

where $\text{int}(a)$ stands for integer part of $a$ and $N = \text{int}(a) + \text{int}(b) + n + n'$ is the degree of the polynomial. We can distinguish four case:

- $a$ and $b$ integers. In this case the integrand polynomial has degree $N = a + b + n + n'$, which can be evaluated using Gauss-Legendre quadrature, i.e.

$$I_j(2a, 2b) = \int_{-1}^{1} dx P_N(x) = \sum_{i=1}^{N_G} \omega_i^{(N_G)} P_N(x_i^{(N_G)}), \quad (A.61)$$

where $\omega_i^{(N_G)}$ and $x_i^{(N_G)}$ are the Gauss-Legendre weights and points.

- $a$ half-integer and $b$ integer. We can write the integral as

$$I_j(2a, 2b) = \int_{-1}^{1} dx \sqrt{1 - x} P_N(x) = 2^\frac{N_G+1}{2} \sum_{i=1}^{2N_G+1} \tilde{\omega}_i^{(2N_G+1)} P_N(2\tilde{x}_i^{(2N_G+1)} - 1), \quad (A.62)$$

where

$$\tilde{\omega}_i^{(2N_G+1)} = 2\epsilon_i^2 \omega_i^{(2N_G+1)}, \quad (A.63)$$

$$\tilde{x}_i^{(2N_G+1)} = 1 - \epsilon_i^2, \quad (A.64)$$

$\tilde{\omega}_i^{(2N_G+1)}$ being the $2N_G + 1$ Gauss-Legendre weights and $\epsilon_i$ the zeros of the $P_{2N_G+1}(x)$ Legendre polynomials.

- $a$ integer and $b$ half-integer. We can write the integral as

$$I_j(2a, 2b) = \int_{-1}^{1} dx \sqrt{1 + x} P_N(x) = 2^\frac{N_G+1}{2} \sum_{i=1}^{2N_G+1} \tilde{\omega}_i^{(2N_G+1)} P_N(1 - 2\tilde{x}_i^{(2N_G+1)}), \quad (A.65)$$

where $\tilde{\omega}_i^{(2N_G+1)}$ and $\tilde{x}_i^{(2N_G+1)}$ are defined in Eqs. (A.63) and (A.64).

- $a$ half-integer and $b$ half-integer. We can write the integral as

$$I_j(2a, 2b) = \int_{-1}^{1} dx \sqrt{1 - x^2} P_N(x) = \sum_{i=1}^{N_G} \omega_i^{(N_G)} P_N(x_i^{(N_G)}), \quad (A.66)$$

where $\omega_i^{(N_G)}$ and $x_i^{(N_G)}$ are the Gauss-Tchebishev weights and points.
The Gauss abscissa and coefficients have the property to give exact results when $N_G = N = \text{int}(a) + \text{int}(b) + n + n'$. The precision is limited only by the internal precision of the computer.

The final expression of the integrals $I_{\mu,\nu}^{\mu',\nu'}$ in terms of $I_j$ and the Wigner 3j coefficients are

\[
I_{1,1}^{\mu,\mu'} = \frac{N_{21}}{16} N_{\mu} N_{\nu} I_2(3 + K_1 + K'_1, 3 + \ell_2 + \ell'_2) I_3(6 + K_2 + K'_2, 1 + \ell_3 + \ell'_3) \\
\times I_4(9 + K_3 + K'_3, 1 + \ell_4 + \ell'_4) I_5(12 + K_4 + K'_4, 1 + \ell_5 + \ell'_5) \\
\times \prod_{i=1}^{5} \delta_{\ell_i,\ell'_i} \prod_{i=2}^{4} \delta_{L_i, L'_i},
\]

(A.67)

\[
I_{1,2}^{\mu,\nu'} = \frac{N_{21}}{16} N_{\mu} N_{\nu} I_2(2 + K_1 + K'_1, 2 + \ell_2 + \ell'_2) I_3(6 + K_2 + K'_2, 1 + \ell_3 + \ell'_3) \\
\times I_4(9 + K_3 + K'_3, 1 + \ell_4 + \ell'_4) I_5(12 + K_4 + K'_4, 1 + \ell_5 + \ell'_5) \\
\times (-1)^{1+L_2} L_1 P_1 L_2 \frac{\ell_1}{\ell_2} \ell_1 \hat{\ell}_2 \hat{\ell}_1 \ell_2 L \hat{L} \\
\times (1 + \ell_1 \ell_2 \ell_3) \left( \begin{array}{c} \ell_1 \\ \ell_2 \\ \ell_3 \\ \ell \end{array} \right) \left( \begin{array}{c} \ell_1 \\ \ell_2 \\ \ell_3 \\ \ell \end{array} \right)
\]

(A.68)

\[
I_{1,3}^{\mu,\mu'} = \frac{N_{21}}{8 \sqrt{2}} N_{\mu} N_{\nu} I_2(2 + K_1 + K'_1, 1 + \ell_2 + \ell'_2) I_3(5 + K_2 + K'_2, 2 + \ell_3 + \ell'_3) \\
\times I_4(9 + K_3 + K'_3, 1 + \ell_4 + \ell'_4) I_5(12 + K_4 + K'_4, 1 + \ell_5 + \ell'_5) \\
\times (-1)^{1+L_3} L_1 P_1 L_2 \hat{L} \hat{L}_2 L \hat{L}_3 \\
\times \left[ \begin{array}{c} \ell_3 \\ \ell_3 \\ \ell_3 \\ \ell \end{array} \right] \left[ \begin{array}{c} \ell_2 \\ \ell_2 \\ \ell_2 \\ \ell \end{array} \right],
\]

(A.69)

\[
I_{1,4}^{\mu,\nu'} = \frac{N_{21}}{8} N_{\mu} N_{\nu} I_2(2 + K_1 + K'_1, 1 + \ell_2 + \ell'_2) I_3(5 + K_2 + K'_2, 2 + \ell_3 + \ell'_3) \\
\times I_4(8 + K_3 + K'_3, 2 + \ell_4 + \ell'_4) I_5(12 + K_4 + K'_4, 1 + \ell_5 + \ell'_5) \\
\times (-1)^{1+L_4} L_1 P_1 L_2 \hat{L} \hat{L}_3 L \hat{L}_4 \\
\times \left[ \begin{array}{c} \ell_4 \\ \ell_4 \\ \ell_4 \\ \ell \end{array} \right] \left[ \begin{array}{c} \ell_3 \\ \ell_3 \\ \ell_3 \\ \ell \end{array} \right],
\]

(A.70)

\[
I_{1,5}^{\mu,\mu'} = \frac{N_{21}}{8 \sqrt{2}} N_{\mu} N_{\nu} I_2(2 + K_1 + K'_1, 1 + \ell_2 + \ell'_2) I_3(5 + K_2 + K'_2, 1 + \ell_3 + \ell'_3) \\
\times I_4(8 + K_3 + K'_3, 1 + \ell_4 + \ell'_4) I_5(11 + K_4 + K'_4, 2 + \ell_5 + \ell'_5) \\
\times (-1)^{1+L_5} L_1 P_1 L_2 \hat{L} \hat{L}_3 L \hat{L}_4 \\
\times \left[ \begin{array}{c} \ell_5 \\ \ell_5 \\ \ell_5 \\ \ell \end{array} \right] \left[ \begin{array}{c} \ell_4 \\ \ell_4 \\ \ell_4 \\ \ell \end{array} \right],
\]

(A.71)

\[
I_{1,6}^{\mu,\nu'} = \frac{N_{21}}{8} N_{\mu} N_{\nu} I_2(1 + K_1 + K'_1, 3 + \ell_2 + \ell'_2) I_3(6 + K_2 + K'_2, 1 + \ell_3 + \ell'_3) \\
\times I_4(9 + K_3 + K'_3, 1 + \ell_4 + \ell'_4) I_5(12 + K_4 + K'_4, 1 + \ell_5 + \ell'_5)
\]
\[ I_{2,3}^{\mu,\nu} = \frac{N_\mu N_\nu}{8\sqrt{2}} I_2 \left( 1 + K_1 + K_1', 2 + \ell_2 + \ell_2' \right) I_3 \left( 5 + K_2 + K_2', 2 + \ell_3 + \ell_3' \right) \]
\[ \times I_5 \left( 9 + K_3 + K_3', 1 + \ell_4 + \ell_4' \right) I_5 \left( 12 + K_4 + K_4', 1 + \ell_5 + \ell_5' \right) \]
\[ \times (-1)^{1+L_3+L_2+\ell_1} \hat{L}_2 \hat{L}_3 \hat{L}_2 \hat{L}_3' \]
\[ \left\{ \ell_3 \ell_3' 1 \right\} \left\{ L_2 \ L_2' \ L_3 \right\} \left\{ L_2' L_2 \ L_3 \right\} \left\{ L_2' L_2 \ \ell_1 \right\} \left\{ 0 \ 0 \ 0 \right\} \left\{ 0 \ 0 \ 0 \right\} \]
\[ \times \delta_{\ell_1 \ell_1'} \delta_{\ell_2 \ell_2'} \delta_{\ell_3 \ell_3'} \delta_{\ell_4 \ell_4'} \delta_{\ell_5 \ell_5'} \delta_{\ell_6 \ell_6'} \delta_{L_3 L_3'} \delta_{L_4 L_4'} \]  
\[ (A.72) \]

\[ I_{2,4}^{\mu,\nu} = \frac{N_\mu N_\nu}{8} I_2 \left( 1 + K_1 + K_1', 2 + \ell_2 + \ell_2' \right) I_3 \left( 5 + K_2 + K_2', 1 + \ell_3 + \ell_3' \right) \]
\[ \times I_5 \left( 8 + K_3 + K_3', 2 + \ell_4 + \ell_4' \right) I_5 \left( 12 + K_4 + K_4', 1 + \ell_5 + \ell_5' \right) \]
\[ \times (-1)^{1+L_4+\ell_3+\ell_3} \hat{L}_2 \hat{L}_3 \hat{L}_2 \hat{L}_3' \]
\[ \left\{ \ell_4 \ell_4' 1 \right\} \left\{ L_3 \ L_3' \ L_4 \right\} \left\{ L_3' L_3 \ \ell_3 \right\} \left\{ L_2' L_2 \ \ell_1 \right\} \left\{ 0 \ 0 \ 0 \right\} \left\{ 0 \ 0 \ 0 \right\} \]
\[ \times \delta_{\ell_1 \ell_1'} \delta_{\ell_2 \ell_2'} \delta_{\ell_3 \ell_3'} \delta_{\ell_4 \ell_4'} \delta_{\ell_5 \ell_5'} \delta_{\ell_6 \ell_6'} \]  
\[ (A.74) \]

\[ I_{2,5}^{\mu,\nu} = \frac{N_\mu N_\nu}{4\sqrt{2}} I_2 \left( 1 + K_1 + K_1', 2 + \ell_2 + \ell_2' \right) I_3 \left( 5 + K_2 + K_2', 1 + \ell_3 + \ell_3' \right) \]
\[ \times I_5 \left( 8 + K_3 + K_3', 1 + \ell_4 + \ell_4' \right) I_5 \left( 11 + K_4 + K_4', 2 + \ell_5 + \ell_5' \right) \]
\[ \times (-1)^{L_3+L_2+\ell_1+\ell_3} \hat{L}_2 \hat{L}_3 \hat{L}_2 \hat{L}_3' \]
\[ \left\{ \ell_5 \ell_5' 1 \right\} \left\{ L_4 \ L_4' \ L_5 \right\} \left\{ L_4' L_4 \ \ell_3 \right\} \left\{ L_2' L_2 \ \ell_1 \right\} \left\{ 0 \ 0 \ 0 \right\} \left\{ 0 \ 0 \ 0 \right\} \]
\[ \times \delta_{\ell_1 \ell_1'} \delta_{\ell_2 \ell_2'} \delta_{\ell_3 \ell_3'} \delta_{\ell_4 \ell_4'} \delta_{\ell_5 \ell_5'} \delta_{\ell_6 \ell_6'} \]  
\[ (A.75) \]

\[ I_{3,3}^{\mu,\nu} = \frac{N_\mu N_\nu}{8} I_2 \left( 1 + K_1 + K_1', 1 + \ell_2 + \ell_2' \right) I_3 \left( 4 + K_2 + K_2', 3 + \ell_3 + \ell_3' \right) \]
\[ \times I_5 \left( 9 + K_3 + K_3', 1 + \ell_4 + \ell_4' \right) I_5 \left( 12 + K_4 + K_4', 1 + \ell_5 + \ell_5' \right) \]
\[ \times \prod_{i=1}^{5} \delta_{\ell_i \ell_i'} \prod_{i=2}^{4} \delta_{L_i L_i'} \]  
\[ (A.76) \]

\[ I_{3,4}^{\mu,\nu} = \frac{N_\mu N_\nu}{4\sqrt{2}} I_2 \left( 1 + K_1 + K_1', 1 + \ell_2 + \ell_2' \right) I_3 \left( 4 + K_2 + K_2', 2 + \ell_3 + \ell_3' \right) \]
\[ \times I_4 \left( 8 + K_3 + K_3', 2 + \ell_4 + \ell_4' \right) I_5 \left( 12 + K_4 + K_4', 1 + \ell_5 + \ell_5' \right) \]
\[ \times (-1)^{L_4+L_3+\ell_4+\ell_3} \hat{L}_3 \hat{L}_4 \hat{L}_3 \hat{L}_4' \]
\[ \left\{ \ell_4 \ell_4' 1 \right\} \left\{ L_3 \ L_3' \ L_4 \right\} \left\{ L_4' L_4 \ \ell_3 \right\} \left\{ L_2' L_2 \ \ell_1 \right\} \left\{ 0 \ 0 \ 0 \right\} \left\{ 0 \ 0 \ 0 \right\} \]
\[ \times \delta_{\ell_1 \ell_1'} \delta_{\ell_2 \ell_2'} \delta_{\ell_3 \ell_3'} \delta_{\ell_4 \ell_4'} \delta_{\ell_5 \ell_5'} \delta_{\ell_6 \ell_6'} \]  
\[ (A.77) \]

\[ I_{3,5}^{\mu,\nu} = \frac{N_\mu N_\nu}{4} I_2 \left( 1 + K_1 + K_1', 1 + \ell_2 + \ell_2' \right) I_3 \left( 4 + K_2 + K_2', 2 + \ell_3 + \ell_3' \right) \]
\[ \times I_4 \left( 8 + K_3 + K_3', 1 + \ell_4 + \ell_4' \right) I_5 \left( 11 + K_4 + K_4', 2 + \ell_5 + \ell_5' \right) \]
\[ \times (-1)^{1+L_2+\ell_4+\ell_4} \hat{L}_3 \hat{L}_4 \hat{L}_3 \hat{L}_4' \]
\[ \left\{ \ell_5 \ell_5' 1 \right\} \left\{ L_4 \ L_4' \ L_5 \right\} \left\{ L_5' L_5 \ \ell_3 \right\} \left\{ L_3' L_3 \ \ell_1 \right\} \left\{ 0 \ 0 \ 0 \right\} \left\{ 0 \ 0 \ 0 \right\} \]  
\[ (A.78) \]
The calculation of the TC implies two main problems we need to consider: (i) the high 
cursion procedure can start following the algorithm showed in Section A.2. The 
be calculated at each step of the recursion is

\[ \delta \]

example, in the case of

\[ \int \]

need to compute. For example, for the case

\[ L \]

integrals are vanishing. This reduces drastically the number of integrals we actually

\[ \lambda \]

integrals on the disk is enormously reduced: the total space occupied by the integrals

\[ \mu \]

which are 4 order of magnitude less. Also the amount of space needed to save the

part of the code computes the integrals

\[ TC \]. The code was written in FORTRAN90 using quadrupole precision. The first

In this section we present some technical details of the code used for computing the

Appendix A. The Transformation Coefficients

\[ N \]

\[ I_{4,4}^{\mu,\mu'} = \frac{N_{21}}{4} N_\mu N_{\mu'} I_2(1 + K + K_1', 1 + \ell_2 + \ell_2') I_3(4 + K_2 + K_2', 1 + \ell_3 + \ell_3') \]

\[ \times I_4(8 + K_3 + K_3', 3 + \ell_4 + \ell_4') I_5(12 + K_4 + K_4', 1 + \ell_5 + \ell_5') \]

\[ \times \prod_{i=1}^{5} \delta_{\ell_i \ell_i'} \prod_{i=2}^{4} \delta_{L_i L_i'}, \quad (A.79) \]

\[ I_{4,5}^{\mu,\mu'} = \frac{N_{21}}{2 \sqrt{2}} N_\mu N_{\mu'} I_2(1 + K + K_1', 1 + \ell_2 + \ell_2') I_3(4 + K_2 + K_2', 1 + \ell_3 + \ell_3') \]

\[ \times I_4(7 + K_3 + K_3', 2 + \ell_4 + \ell_4') I_5(11 + K_4 + K_4', 2 + \ell_5 + \ell_5') \]

\[ \times (-1)^{L+L_4+L_5+L_3} \delta_{\ell_4 \ell_4'} \delta_{\ell_5 \ell_5'} L_4 L_5 \]

\[ \times \left\{ \ell_4, L_4, L \right\} \left\{ \ell_5, L_5, L_3 \right\} \left( \begin{array}{ccc} 1 & \ell_4' & \ell_4 \\ 0 & 0 & 0 \end{array} \right) \left( \begin{array}{ccc} 1 & \ell_5' & \ell_5 \\ 0 & 0 & 0 \end{array} \right) \]

\[ \times \delta_{\ell_1 \ell_1'} \delta_{\ell_2 \ell_2'} \delta_{\ell_3 \ell_3'} \delta_{L_2 L_2'} \delta_{L_3 L_3'}, \quad (A.80) \]

\[ I_{5,5}^{\mu,\mu'} = \frac{N_{21}}{2} N_\mu N_{\mu'} I_2(1 + K + K_1', 1 + \ell_2 + \ell_2') I_3(4 + K_2 + K_2', 1 + \ell_3 + \ell_3') \]

\[ \times I_4(7 + K_3 + K_3', 1 + \ell_4 + \ell_4') I_5(10 + K_4 + K_4', 3 + \ell_5 + \ell_5') \]

\[ \times \prod_{i=1}^{5} \delta_{\ell_i \ell_i'} \prod_{i=2}^{4} \delta_{L_i L_i'}, \quad (A.81) \]

where \( N_{21} = 1/2^{21} \) and

\[ N_\mu = \prod_{j=2}^{5} N_{\nu_j K_{j-1}}. \quad (A.82) \]

A.2.2 Details of the implementation

In this section we present some technical details of the code used for computing the

TC. The code was written in FORTRAN90 using quadrupole precision. The first

part of the code computes the integrals \( I_{ij}^{\mu,\mu'} \) and stores them in files. If we define

\( N_{K,L} \) as the number of states \( \mu \) for a give value of \( K \) and \( L \), the number of integrals

to be calculated at each step of the recursion is

\[ N_I = 15 N_{K+2,L} N_{K,L}. \quad (A.83) \]

Due to the \( \delta \)-functions and the Wigner 3j “triangular conditions”, many of these
integrals are vanishing. This reduces drastically the number of integrals we actually
need to compute. For example, for the case \( L = 2 \) and \( K = 12 \), the number of integrals is

\( N_I \approx 8.3 \times 10^{10} \). However the number of non-zero integrals is 10,099,724
which are 4 order of magnitude less. Also the amount of space needed to save the
integrals on the disk is enormously reduced: the total space occupied by the integrals
used in this work, saved in quadrupole precision, is only 3.7 GB. Moreover, the
explicit implementation of the vanishing condition combined with the parallelization
of the calculation on the states \( \mu \) reduced drastically the computing time. For
example, in the case of \( L = 2 \) and \( K = 12 \), the calculation of the integrals takes
\(~15 \) minutes on a 48-core CPU with 2.10 GHz.

In the second part of the code we select a state \( \lambda \) [see Eq. (A.14)] and the rec-
ursion procedure can start following the algorithm showed in Section A.2. The

calculation of the TC implies two main problems we need to consider: (i) the high
number of permutations (360) increase dramatically the time required for the computation, and (ii) at each step we need to store all the coefficients $c_{KL,p}^{K\mu,\mu'}$ needed then for the case $K + 2$. The first problem was easily overcome by parallelizing on the permutations which are independent from each other. The second problem is related to the memory needed for storing all the coefficients. If we want to compute the coefficients for the case $K + 2$ for a given $\lambda$, we need to store the coefficients $c_{KL,p}^{K\mu,\mu'}$ for all the combinations of $n_2, n_3, n_4, n_5$ and for all the permutations. If we define $N = (K - \ell_{\text{sum}})/2$, where $\ell_{\text{sum}} = \ell_1 + \ell_2 + \ell_3 + \ell_4 + \ell_5$, the number of combinations of $n_2, n_3, n_4, n_5$ is given by

$$N_n(K, \ell_{\text{sum}}) = \frac{1}{6}(N + 1)(N^2 + 5N + 6).$$  \hspace{1cm} (A.84)

Multiplying this number for the 360 permutations, the number of coefficients $N_{K,L}$ of the given state $\mu$ and the 16 byte occupied by each coefficient, we have the total memory needed for the storage at each recursion step, namely

$$M[\text{GB}] = 16 \times \frac{360 \times N_{K,L} \times N_n(K, \ell_{\text{sum}})}{1024^3}. \hspace{1cm} (A.85)$$

For example, if we want to compute the coefficients $c_{12,0}^{12,0,p}$ where the states $\mu$ have $\ell_{\text{sum}} = 2$, we need the corresponding coefficients at $K = 10$. Considering that $N_{10,2} = 30,525$, using Eqs. (A.84) and (A.85), the memory required for the storage is $\sim 6$ GB which can be easily managed by standard supercomputers. The possibility of working only with the single core memory reduces enormously the computing time. However, as it can be seen from Eq. (A.84), the memory requirement is proportional to $N_{K,L}$. Therefore it grows exponentially for increasing $K$. Hence, for future applications in which we plan to increase $K$, we will be obliged to store the coefficients on the disk reducing drastically the performances of the code, or implement more sophisticated codes, using a distributed memory over different cores.

As regarding the precision, the main source of error was found to be in the zero case of the recursion. All the other loss of precision are due to the round-off of the computer. In order to have a run-time check on the precision, we use the orthonormal properties of the HH functions which requires that

$$C_{\mu}^p = \sum_{\mu'} \left( c_{\mu;\mu'}^{K\mu,\mu'} \right)^2 = 1. \hspace{1cm} (A.86)$$

In particular we impose that

$$|C_{\mu}^p - 1| < 10^{-28}, \hspace{1cm} (A.87)$$

condition fulfilled by each state $\mu$ we have considered.

### A.3 Orthogonalization procedure

The sum over the permutation present in Eq. (2.57) generates a strong redundancy that must be eliminated as already discussed in Chapter 2. In this section we present the procedure we used to individuate the independent states. The orthogonalization process is the real bottleneck of the construction of the 6-body wave function within the HH formalism. Let us suppose to have already defined a set of states that are linear independent and we are checking a new state. There are two possibilities: or the new state is completely dependent on the orthogonal basis or the new state has an
orthogonal component to the basis we have calculated so far, and we have to include it. However, this orthogonal component can be very small, and therefore, very hard to identify. This means that it can happen very easily to not identify some orthogonal component due to the numerical round-off precision of the computer. This problem grows exponentially increasing the value of the grandangular momentum \( K \), since smaller and smaller components must be identified.

This problem forces us to improve the precision both from the algorithmic and the implementation point of view. As already discussed, we implemented the code in quadrupole precision (32 digits) in order to have less round-off errors. As regarding the algorithm, typically the Gram-Schmidt method is usually used to orthogonalization of a basis. In our case, we implement an algorithm using the LINPACK libraries which are based on Gaussian elimination. The algorithm works as follow: (i) selected an order of the states, we keep as first state the first that has non-zero norm. (ii) Let us suppose we have already individuated \( M \) independent states and let us define the matrix

\[
N_{KLSTJ\pi}^M = \begin{pmatrix}
N_{\alpha_1,\alpha_1} & \cdots & N_{\alpha_1,\alpha_M} \\
\vdots & \ddots & \vdots \\
N_{\alpha_M,\alpha_1} & \cdots & N_{\alpha_M,\alpha_M}
\end{pmatrix},
\]

where

\[
N_{\alpha_i,\alpha_j} = \sum_{\alpha''} (A_{KLSTJ\pi}^{\alpha,\alpha''})^* A_{KLSTJ\pi}^{\alpha'',\alpha_j}.
\]

(A.89)

Considering now a new state \( \alpha_{M+1} \), let us compute the norms \( N_{\alpha_{M+1},\alpha_i} \) with all the \( M \) independent states \( \alpha_i \). (iii) The new norm matrix of dimensions \((M+1)\times(M+1)\) is then

\[
N_{KLSTJ\pi}^{M+1} = \begin{pmatrix}
N_{\alpha_1,\alpha_1} & \cdots & N_{\alpha_1,\alpha_M} & N_{\alpha_1,\alpha_{M+1}} \\
\vdots & \ddots & \vdots & \vdots \\
N_{\alpha_M,\alpha_1} & \cdots & N_{\alpha_M,\alpha_M} & N_{\alpha_M,\alpha_{M+1}} \\
N_{\alpha_{M+1},\alpha_1} & \cdots & N_{\alpha_{M+1},\alpha_M} & N_{\alpha_{M+1},\alpha_{M+1}}
\end{pmatrix},
\]

(A.90)

which is inverted using LINPACK libraries, modified to work in quadrupole precision and in parallel. From this we get the condition number \( R \) which tells us if the matrix can be inverted or not. (iv) If \( R > R_{\text{min}} \), where \( R_{\text{min}} = 10^{-30} \), the matrix is invertible and so we put the new state in the independent basis, in the other case the matrix is not invertible and we discard it. We select \( R_{\text{min}} = 10^{-30} \) in order to be conservative, compared to the precision of the computer (i.e. \( 10^{-32} \)). The procedure is then repeated for all the states of given \( KLSTJ\pi \). This approach permits to individuate very small orthogonal components when we add new states. For example for \( K = 12 \) and \( LSTJ\pi = 0101+ \), we were able to find independent states up to value of \( R \sim 10^{-18} \), which would be impossible in double precision.

In the implementation of the orthogonalization procedure it is important to consider the time consumption, due to the large amount of states we need to test. Moreover, the parallelization results not trivial because the algorithm can check only one state at a time. Indeed at the end, this part results to be the most inefficient part of the code. For example, if we consider \( L = 0 \) and a given \( \lambda \), the time needed for computing all the TC for all the states \( \alpha \) up to \( K = 12 \) results to be \( \sim 20 \) minutes without the orthogonalization procedure. On the other hand, if we want to identify the independent states through the orthogonalization procedure, the time spent is more than 10 hours. Much of this time is used to invert the norm matrix. In fact,
while much of the computation time of the norm matrix can be saved by storing the norm matrix element, the inversion of the norm matrix given in Eq. (A.90) has to be performed every time. Therefore, only a preliminary identification of the orthogonal states can really improve the algorithm efficiency. On the other hand, this orthogonalization has to be done only once.
Appendix B

Transformation of the HH states

The calculation of some observables can be performed more easily and precisely by changing the definitions of the Jacobi vectors and the hypercoordinates compared to the standard ones defined in Eqs. (2.4) and (2.7). This implies that we need to express the HH-spin-isospin basis functions defined in Eq. (2.47) according to the new coordinate definition. This transformation can be done by using particular TC, which we discuss in this appendix.

From the computational point of view, the most efficient way to perform this transformation is to compute separately the TC for the spatial, spin, and isospin parts for each permutation, and then sum over the permutations, as already discussed in Appendix A. The transformation we are considering involves only the spatial coordinates, while the spin-isospin states are the same as considered in Appendix A, so for spin and isospin we can proceed as already discussed. The only part we will modify is the spatial part for which we define new coefficients

\[ Y_{KLM}^{\mu} (\Omega_5^p) = \sum_{\mu'} c_{KL,p}^{\mu \mu'} Y_{KLM}^{\mu'} (\Omega_X) , \]  

where \( \Omega_5^p \) represents a generic permutation of the standard Jacobi coordinates, while \( \Omega_X \) represents a generic definition of the Jacobi vectors in the reference permutation and \( c_{KL,p}^{\mu \mu'} \) are the coefficients which permit to transform the HH states defined in the Jacobi coordinates \( \Omega_5^p \) to the ones defined in the coordinates \( \Omega_X \). It is clear that only small modification of the algorithm presented in Appendix A are really needed. In this Appendix we will discuss only this small modifications for the case of the change of variables for the calculation of the quadrupole moment and for the scattering case.

B.1 From the standard variables to “X” variables

In this Section we will discuss the calculation of the coefficients \( c_{KL,p}^{\mu \mu'} \) defined in Eq. (B.1), where the “X” stands for the set “Q” in the case of the quadrupole moment [see Eqs. (3.41) and (3.42)] or the set “B” in the case of the scattering states [see Eqs. (2.5) and (G.1)]. By following Appendix A, the coefficients are obtained by using

\[ c_{KL,p}^{X \mu \mu'} = \int d\Omega_X \left[ Y_{\mu}^{KL,M} (\Omega_X) \right]^\dagger Y_{\mu'}^{KL,M} (\Omega_5^p) , \]  

from which it is possible to derive the recursion relations. They turn out to be exactly identical to the ones derived in Appendix A, because we are applying the recursion formula of the Jacobi polynomials. The only changes are:
1) the integration must be done over the “X” variables, therefore the integrals \( I_{\mu,\mu'}^{ij} \) result

\[
I_{\mu,\mu'}^{ij} = \int d\Omega_X \left[ Y_{\mu}^{K+2LM}(\Omega_X) \right]^\dagger \frac{x_i^X \cdot x_j^X}{\rho^2} Y_{\mu'}^{KLM}(\Omega_X). \tag{B.3}
\]

2) The coefficients \( \Gamma_{i,j} \) of Eq. (A.20) must be re-evaluated by inverting the equation

\[
(x_{lp})^2 = \sum_{i,j} \Gamma_{i,j}^{p\rightarrow X}(l) x_i^X \cdot x_j^X. \tag{B.4}
\]

All the other steps remain exactly the same.

### B.2 From the scattering to the standard Jacobi

This section is dedicated to the calculation of the coefficients \( c_{KL,Bp\rightarrow 1}^{\mu,\mu'} \) defined such that

\[
Y_{\mu}^{KLM}(\Omega_{Bp}) = \sum_{\mu'} c_{KL,Bp\rightarrow 1}^{\mu,\mu'} Y_{\mu'}^{KLM}(\Omega_5), \tag{B.5}
\]

where \( \Omega_{Bp} \) represents a generic permutation of the coordinates defined in Eq. (2.5), with the hyperangular variables defined in Eq. (G.1), while \( \Omega_5 \) represent the coordinate in the standard definition and in the reference permutation. By following Appendix A, the coefficients are obtained by

\[
c_{KL,Bp\rightarrow 1}^{\mu,\mu'} = \int d\Omega_5 \left[ Y_{\mu}^{KLM}(\Omega_5) \right]^\dagger Y_{\mu'}^{KLM}(\Omega_{Bp}), \tag{B.6}
\]

from which we derive the new recursion relations. From the formal point of view, the result is identical to the one given in Appendix A. However, it is fundamental to redefine the normalization of the recursion factors given in Eq. (A.18) by taking care of the new definition of the quantum number \( K_i \) and \( \nu_i \) [see Eqs. (G.4) and (G.5)]. By using the new definitions we obtain

\[
N_{\ell_1,...,\ell_N}^{\eta_1,...,\eta_N} = N_{\ell_4,\nu_2}^{\eta_4,\nu_2} N_{\ell_5,\nu_2}^{\eta_5,\nu_2} N_{\ell_1,\nu_4}^{\eta_1,\nu_4} N_{\ell_2,\nu_5}^{\eta_2,\nu_5}, \tag{B.7}
\]

where \( N_{\eta_i,K_{i-1}}^{\ell_i,\nu_i} \) are defined in Eq. (A.12). All the rest remains exactly identical to what reported in Appendix A.
Appendix C

Useful formulas for the matrix elements

In this Appendix we give the explicit formula for the calculation of the kinetic energy matrix elements (Section C.1) and the calculation of the TC in the $jj$-coupling (Section C.2).

C.1 Kinetic energy matrix element

The kinetic energy matrix element given in Eq. (2.74) contains the integral on the hyperradius, that for a generic number of particle $A$ reads

$$T_{l,l'} = -\frac{\hbar^2}{m} \int_0^\infty d\rho \rho^{3N-1} f_l(\rho) \left( \frac{\partial^2}{\partial \rho^2} + \frac{3N-1}{\rho} \frac{\partial}{\partial \rho} + \frac{K(K+3N-2)}{\rho^2} \right) f_{l'}(\rho), \quad (C.1)$$

where $N = A - 1$, $D = 3N$ and $f_l(\rho)$ are defined in Eq. (2.62). Using the properties of the Laguerre polynomials, Eq. (C.1) can be cast in the form [69]

$$T_{l,l'} = \frac{\hbar^2 \gamma^2}{m} \left[ (l' + K(K + 3N - 2)) I_{l,l'}^{(2)} + \left( l' + \frac{3N-1}{2} \right) I_{l,l'}^{(1)} \right. \left. - \sqrt{l'(l' + 3N - 1)} I_{l,l'-1}^{(2)} - \frac{1}{4} \delta_{l,l'} \right], \quad (C.2)$$

where

$$I_{l,l'}^{(1)} = \frac{N_l N_{l'}}{\gamma^D} \int_0^{+\infty} dx x^{D-2} e^{-x} L^{(D-1)}(x) L^{(D-1)}_{l'}(x), \quad (C.3)$$

$$I_{l,l'}^{(2)} = \frac{N_l N_{l'}}{\gamma^D} \int_0^{+\infty} dx x^{D-3} e^{-x} L^{(D-1)}(x) L^{(D-1)}_{l'}(x), \quad (C.4)$$

and

$$N_l = \gamma^{D/2} \sqrt{\frac{l!}{(l + D - 1)!}}, \quad (C.5)$$

The integrals given in Eqs. (C.3) and (C.4) can be obtained analytically.

C.2 $jj$-coupling scheme

In this Section we present the connection between the so called $jj$-coupling scheme defined in Eq. (2.78) and the definition given in Eq. (2.49). By rewriting a state $\alpha$
Appendix C. Useful formulas for the matrix elements

in the $jj$-coupling scheme we obtain

$$\Phi^K_{\ell L S T J \pi}^{\alpha}(i, j, k, l, m, n) = \sum_{j_1 j_2 j_3 j_{12}} C^{j_1 j_2 j_3 j_{12}}_{\ell_4 \ell_5 L_4 L_3 S_2 S_3 S_5 S_3 S_5 S_5 S_\xi} \Xi^K_{\nu J \pi}^{\tau}(i, j, k, l, m, n), \quad (C.6)$$

where the coefficient $C^{j_1 j_2 j_3 j_{12}}_{\ell_4 \ell_5 L_4 L_3 S_2 S_3 S_5 S_5 S_5 S_\xi}$ explicitly reads

$$C^{j_1 j_2 j_3 j_{12}}_{\ell_4 \ell_5 L_4 L_3 S_2 S_3 S_5 S_5 S_5 S_\xi} = \hat{L}_4 \hat{S}_3 \hat{S}_5 \hat{S}_j \hat{j}_1 \hat{j}_2 \hat{j}_3 \hat{j}_{12} \times \sum_{\lambda} (2\lambda + 1) \left\{ \begin{array}{ccc} L_3 & \ell_4 & L_4 \\ \ell_5 & L & \lambda \end{array} \right\} \left\{ \begin{array}{ccc} \ell_4 & \ell_5 & \lambda \\ S_2 & 1/2 & S_3 \end{array} \right\} \left\{ \begin{array}{ccc} \lambda & L_3 & L \\ S_3 & S_5 & S \end{array} \right\}, \quad (C.7)$$

and $\Xi^K_{\nu J \pi}^{\tau}(i, j, k, l, m, n)$ is defined in Eq. (2.78) for the reference permutation $(1, 2, 3, 4, 5, 6)$. In Eq. (C.7) we have used the notation $\hat{l} = \sqrt{2l + 1}$. Note that these coefficients do not depend on the permutation. In such a way the state $\Psi^K_{\ell L S T J \pi}^{\alpha}$ of Eq. (2.77) results

$$\Psi^K_{\ell L S T J \pi}^{\alpha} = \sum_{\alpha'} A^K_{\ell L S T J \pi}^{\alpha, \alpha'} \sum_{j_1 j_2 j_3 j_{12}} C^{j_1 j_2 j_3 j_{12}}_{\ell_4 \ell_5 L_4 L_3 S_2 S_3 S_5 S_5 S_3 S_5 S_5 S_\xi} \Xi^K_{\nu J \pi}^{\tau}(1, 2, 3, 4, 5, 6)$$

$$= \sum_{\nu} \sum_{L_4 S_3} A^K_{\ell L S T J \pi}^{\alpha, \alpha'} C^{j_1 j_2 j_3 j_{12}}_{\ell_4 \ell_5 L_4 L_3 S_2 S_3 S_5 S_5 S_3 S_5 S_5 S_\xi} \Xi^K_{\nu J \pi}^{\tau}(1, 2, 3, 4, 5, 6), \quad (C.8)$$

where we transformed the sum over $\alpha'$ defined in Eq. (2.50) in the sum over $\nu$ defined in Eq. (2.79). Therefore

$$B^K_{\ell L S T J \pi}^{\alpha, \nu} = \sum_{L_4 S_3} A^K_{\ell L S T J \pi}^{\alpha, \alpha'} C^{j_1 j_2 j_3 j_{12}}_{\ell_4 \ell_5 L_4 L_3 S_2 S_3 S_5 S_5 S_3 S_5 S_5 S_\xi} \cdot \quad (C.9)$$
Appendix D

Lanczos algorithm

The eigenvalue problem presented in Eq. (2.66) is solved using an iterative algorithm based on the Lanczos approach. In particular, we use the approach invented by Cullum and Willoughby [70], which allows for a limited use of the computer memory. In this appendix we present the main points of this algorithm.

Eq. (2.66) can be rewritten as

\[(T + V) c = E N c,\]

where \(T\) is the kinetic energy matrix, \(V\) is the potential energy matrix, \(N\) is the norm matrix, and \(E\) and \(c\) are respectively the eigenvalue and the eigenstate. Moreover, we define \(M\) as the dimension of the matrices. In order to use the Lanczos algorithm we need to transform the generalized eigenvalue problem in a standard eigenvalue problem. To this aim, we use the Cholesky decomposition on the norm matrix \(N\), namely

\[N = U U^\dagger,\]

so that we can rewrite Eq. (D.1) as

\[\left(\tilde{T} + \tilde{V}\right) \tilde{c} = E \tilde{c},\]

where \(\tilde{T} = U^{-1}T(U^\dagger)^{-1}\), \(\tilde{V} = U^{-1}V(U^\dagger)^{-1}\) and \(\tilde{c} = U^\dagger c\). The calculation of \(\tilde{T}\) and \(\tilde{V}\) results to be simplified, because the matrix \(N\), and therefore the matrix \(U^{-1}\), are block diagonal.

The problem of finding the eigenvalue and the eigenvector of Eq. (D.3) can be solved iteratively. Let us select a possible value of the eigenvalue \(E_1\). Eq. (D.3) reduces to the form

\[\left(\tilde{T} - E_1\right) \tilde{c} = -\lambda(E_1) \tilde{V} \tilde{c},\]

where \(\lambda(E_1)\) is equal to 1 only if \(E_1\) is the exact eigenvalue of Eq. (D.3). Rewriting Eq. (D.4) as

\[\left(\tilde{T} - E_1\right)^{-1}(-\tilde{V}) \tilde{c} = \frac{1}{\lambda(E_1)} \tilde{c},\]

the idea now is to select \(E_1\) so that \(\lambda(E_1) = 1\). The problem is now reduced to find the eigenvalues of \(\left(\tilde{T} - E_1\right)^{-1}(-\tilde{V})\).

We can now use the Lanczos algorithm to compute the value \(\lambda(E_1)\) in the form presented in Ref. [70]. Let us select a value of \(E_1\) and try to solve the system

\[A(E_1) \tilde{c} = \frac{1}{\lambda(E_1)} \tilde{c},\]

where \(A(E_1) = \left(\tilde{T} - E_1\right)^{-1}(-\tilde{V})\). In order to do that, we build a biorthonormal basis with dimension \(\nu \ll M\). First of all we select two initial vectors \(a_1\) and \(b_1\) of
dimension $M$ such that $b_1^i a_1 = 1$. The rest of the not normalized vector of the basis (with a tilde) are defined by

$$
\begin{align*}
\tilde{a}_{i+1} &= A(E_1)a_i - \alpha_i a_i - \beta_i a_{i-1}, \\
\tilde{b}_{i+1} &= A(E_1)^\dagger b_i - \alpha_i b_i - \gamma_i b_{i-1},
\end{align*}
$$

with

$$
\alpha_i = b_i^\dagger A(E) a_i, \quad \gamma_i = \sqrt{\tilde{b}_i^\dagger \tilde{a}_i}, \quad \beta_i = \frac{\tilde{b}_i^\dagger \tilde{a}_i}{\sqrt{\tilde{b}_i^\dagger \tilde{a}_i}},
$$

where the vectors $a_0 = b_0 = 0$ by definition. The vectors $\tilde{a}_i$ and $\tilde{b}_i$ are then orthonormalized by imposing $b_{i+1}^i a_{i+1} = 1$ and so we obtain

$$
\begin{align*}
a_{i+1} &= \frac{\tilde{a}_{i+1}}{\sqrt{|\tilde{b}_{i+1}^\dagger \tilde{a}_{i+1}|}}, \\
b_{i+1} &= \frac{\tilde{b}_{i+1}}{\sqrt{|\tilde{b}_{i+1}^\dagger \tilde{a}_{i+1}|}}.
\end{align*}
$$

The eigenvector $\tilde{c}$ can be expanded in term of the basis vector $a_i$, namely

$$
\tilde{c} = \sum_{i=1}^{\nu} \epsilon_i a_i,
$$

and so the eigenproblem of Eq. (D.6) can be rewritten as

$$
\sum_{i=1}^{\nu} \epsilon_i A(E_1)a_i = \frac{1}{\lambda(E_1)} \sum_{i=1}^{\nu} \epsilon_i a_i.
$$

If now we project this equation on $b_j^\dagger$ and we use Eq. (D.7) combined with the orthonormal properties of the basis, it results

$$
\sum_{i=1}^{\nu} \epsilon_i (\delta_{j,i+1} \gamma_{i+1} + \alpha_i \delta_{j,i} + \beta_i \delta_{j,i-1}) = \frac{1}{\lambda(E_1)} \epsilon_j
$$

which is a new eigenvalue problem almost equivalent to Eq. (D.6), where the eigenvector is $\epsilon$ and the eigenvalue is $1/\lambda(E_1)$. In a more familiar form, it can be written as

$$
\begin{pmatrix}
\alpha_1 & \beta_2 & 0 & 0 & \ldots & 0 \\
\gamma_2 & \alpha_2 & \beta_3 & 0 & \ldots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \ldots & 0 & \gamma_{\nu-1} & \alpha_{\nu-1} & \beta_\nu \\
0 & \ldots & 0 & \gamma_\nu & \alpha_\nu
\end{pmatrix}
\begin{pmatrix}
\epsilon_1 \\
\epsilon_2 \\
\vdots \\
\epsilon_{\nu-1} \\
\epsilon_\nu
\end{pmatrix} = \frac{1}{\lambda(E_1)}
\begin{pmatrix}
\epsilon_1 \\
\epsilon_2 \\
\vdots \\
\epsilon_{\nu-1} \\
\epsilon_\nu
\end{pmatrix}.
$$

The eigenvalue obtained from this equation are approximately the eigenvalue of Eq. (D.6). Increasing the dimension of the biorthonormal basis $\nu$, the value of the eigenvalue becomes closer and closer to the real value. Usually, a value of $\nu = 20-30$ is enough to obtain a good accuracy.

In order to obtain the eigenvalue $E$ of Eq. (D.1) we need to extrapolate it. We select two energies $E_1$ and $E_2$ and we compute the corresponding $\lambda(E_1)$ and $\lambda(E_2)$ by using the algorithm explained above. At this point we evaluate a third values $E_3$.
using a linear extrapolation,

\[ E_{i+1} = E_i + \frac{E_i - E_{i-1}}{\lambda(E_i) - \lambda(E_{i-1})} [1 - \lambda(E_i)] , \]  

and using the Lanczos algorithm a new value \( \lambda(E_3) \). The process is then iterated until \( |\lambda(E_i) - 1| < \eta \), where \( \eta \) is usually \( 10^{-5} \). The number of iterations needed for reach such accuracy depends drastically on the choice of \( E_1 \) and \( E_2 \). The furthest they are from the real eigenvalue \( E \), the largest will be the number of iterations needed to obtain the desired precision.

On the other hand this algorithm results to be very time-saving, because there are no matrix operations except for the inversion of \( (\tilde{T} - E_i) \), which in any case results very fast because this matrix is block diagonal. All the other operations in the algorithm are vector-vector or matrix-vector products which are very easy to parallelize. For example, the calculation of the eigenstate of a matrix of size \( M \sim 70,000 \) using the parallelized LAPACK libraries requires a computational time is \( \sim 4 \) hours. The same system solved with the parallelized version of this algorithm requires \( \sim 30 \) minutes.
Appendix E

Validation of the results

In this appendix we perform a benchmark with the results presented in Ref. [80] obtained with the NSHH approach. Moreover, we present the convergence of the results as function of the maximum number of Laguerre polynomials \( (l_{\text{max}}) \) used to expand the hyperradial part of the \(^6\text{Li} \) wave function. We also show the stability of the results by changing the parameter \( \gamma \) [see Eq. (2.62)].

In order to perform these tests, we use the Volkov potential

\[
V(r) = V_R e^{-r^2/R_1^2} + V_A e^{-r^2/R_2^2}, \tag{E.1}
\]

where \( V_R = 144.86 \) MeV, \( R_1 = 0.82 \) fm, \( V_A = -83.34 \) MeV and \( R_2 = 1.6 \) fm. Moreover, for the kinetic energy we consider \( \hbar^2/m = 41.47 \) MeV fm\(^2 \). Since, the Volkov potential is a central potential, it does not couple the different partial wave components of the wave function. Therefore, we consider only the \( L = 0, S = 1 \) and \( T = 0 \) component. In such a way, we are exactly in the same conditions of Ref. [80]. Since, in both the works we are using the same expansions basis, we expect to obtain exactly the same results.

In Table E.1 we report the binding energy of the bound state of \( A = 6 \) as function of the grandangular momentum \( K \) and the maximum total angular momentum of the states used in the basis expansion, i.e. \( \ell_{\text{sum}} = \ell_1 + \ell_2 + \ell_3 + \ell_4 + \ell_5 \). For this calculation we use \( l_{\text{max}} = 16 \) and \( \gamma = 4 \) fm\(^{-1} \). As it can be seen from the table, if we use only the HH states with \( \ell_{\text{sum}} = 0 \) we are not able to reproduce the results of Ref. [80]. The missing energy is due to the fact we are not considering the states with \( \ell_{\text{sum}} = 2 \) (states with \( \ell_{\text{sum}} > 2 \) does not appear for \( K \leq 12 \)). When we add them, our results coincide with those of Ref. [80] except for the case \( K = 12 \), for which a \( 2 \) keV difference remains. Indeed, while in Ref. [80] the entire HH basis is used, in our calculation for \( K = 10 \) and 12 we need to perform a precision

| \( K \) | \( \ell_{\text{sum}} = 0 \) | \( \ell_{\text{sum}} = 2 \) | Ref. [80] |
|---|---|---|---|
| 2 | -61.142 | -61.142 | -61.142 |
| 4 | -62.015 | -62.015 | -62.015 |
| 6 | -63.377 | -63.377 | -63.377 |
| 8 | -64.415 | -64.437 | -64.437 |
| 10 | -65.310 | -65.354 | -65.354 |
| 12 | -65.823 | -65.884 | -65.886 |

Table E.1: Binding energy of the bound state of \( A = 6 \) as function of the grandangular momentum \( K \) obtained with the Volkov potential. The first two columns are the results obtained in this work considering states up with \( \ell_{\text{sum}} = 0 \) and \( \ell_{\text{sum}} = 2 \) respectively. In the third column we report the results of Ref. [80].
truncation. In our approach we need to eliminate the states with tiny orthogonal component (see Section A.3 for more details), since the numerical precision on this small components is not sufficient, when we diagonalize the Hamiltonian. If we leave these states, the numerical errors produced by the inversion on the norm matrix [see Eq. (D.1)] generates spurious bound states that we cannot control. Therefore, we perform a truncation of the basis in the case $K = 10$ and $K = 12$, which avoids the generation of these spurious bound states. We want to remark that despite this truncation, only $2$ keV are missing for $K = 12$, well below the precision of the convergence on $K$. The same truncation is used also for the results presented in the main text.

| $K$ | $\gamma = 2$ fm$^{-1}$ | $\gamma = 3$ fm$^{-1}$ | $\gamma = 4$ fm$^{-1}$ | $\gamma = 5$ fm$^{-1}$ |
|-----|------------------|------------------|------------------|------------------|
| 2   | $-61.13930$      | $-61.14173$      | $-61.14179$      | $-61.14179$      |
| 4   | $-62.01158$      | $-62.01498$      | $-62.01505$      | $-62.01505$      |
| 6   | $-63.37271$      | $-63.37729$      | $-63.37738$      | $-63.37738$      |
| 8   | $-64.43157$      | $-64.43714$      | $-64.43725$      | $-64.43725$      |
| 10  | $-65.34743$      | $-65.35338$      | $-65.35356$      | $-65.35356$      |
| 12  | $-65.87837$      | $-65.88431$      | $-65.88443$      | $-65.88444$      |

Table E.2: Binding energy of the bound state of $A = 6$ as function of the grandangular momentum $K$ obtained with the Volkov potential by varying the parameter $\gamma$. For all the cases we use $l_{\text{max}} = 16$.

In Table E.2 we show the values of the binding energy as function of $K$ obtained, using different values of the parameter $\gamma$, with $l_{\text{max}} = 16$. As it can be seen, the results are very stable changing $\gamma$, and we obtain five digits of stability after the decimal point for values of $\gamma = 4 - 5$ fm$^{-1}$. We performed a similar analysis also for the other potentials used in this work, and the value $\gamma = 4$ fm$^{-1}$ turned out to be the natural choice in all cases.

| $K$ | $l_{\text{max}} = 4$ | $l_{\text{max}} = 8$ | $l_{\text{max}} = 12$ | $l_{\text{max}} = 16$ |
|-----|------------------|------------------|------------------|------------------|
| 2   | $-60.9702$       | $-61.1403$       | $-61.1418$       | $-61.1418$       |
| 4   | $-61.8599$       | $-62.0129$       | $-62.0150$       | $-62.0150$       |
| 6   | $-63.2324$       | $-63.3745$       | $-63.3773$       | $-63.3774$       |
| 8   | $-64.2347$       | $-64.4336$       | $-64.4372$       | $-64.4373$       |
| 10  | $-65.1077$       | $-65.3495$       | $-65.3534$       | $-65.3536$       |
| 12  | $-65.6212$       | $-65.8804$       | $-65.8843$       | $-65.8844$       |

Table E.3: Binding energy of the bound state of $A = 6$ as function of the grandangular momentum $K$ obtained with the Volkov potential by varying the maximum number of Laguerre polynomials ($l_{\text{max}}$) used to expand the hyperradial part of the function. For all the cases we use $\gamma = 4$ fm$^{-1}$.

In Table E.3 we study the convergence of the binding energy as function of $l_{\text{max}}$. For these results we use $\gamma = 4$ fm$^{-1}$. As it can be seen by inspecting the table, we obtain the convergence to $1$ keV with $l_{\text{max}} = 16$. We studied also the convergence in the case of the SRG and the NNLO$_{\text{sat}}$(NN) potentials, obtaining similar results.
Appendix F

Details of the calculation of $^6$Li electromagnetic static properties

In this appendix we discuss the explicit method we have used to calculate the mean value of the charge radius, the magnetic dipole moment and the electric quadrupole moment of $^6$Li. The definition of the mean value of a generic operator $\hat{O}$ for $^6$Li is

$$\langle O \rangle = \langle \Psi_{^6\text{Li}} | \hat{O} | \Psi_{^6\text{Li}} \rangle,$$  \hspace{1cm} (F.1)

where $\hat{O}$ is $\hat{r}_c^2$ defined in Eq. (3.24), $\hat{S}_z$ and $\hat{L}_z$ defined in Eqs. (3.31) and (3.32), $\hat{Q}$ as defined in Eq. (3.38). Finally, $\Psi_{^6\text{Li}}$ is the $^6$Li wave function as defined in Eq. (2.61). The computational approaches presented in this Appendix were validated performing the same calculations with Monte Carlo integration techniques.

F.1 Charge radius

We need to compute the mean value of the proton point charge radius, which, by using Eq. (3.28), translates into

$$\langle r_\alpha^2 \rangle_p = \frac{1}{12} \langle \Psi_{^6\text{Li}} | \rho^2 | \Psi_{^6\text{Li}} \rangle_{\Omega, \rho},$$  \hspace{1cm} (F.2)

where $\rho$ is the hyperradius and $\langle \cdots \cdots \cdots \rho \rangle_{\Omega, \rho}$ represents the integral over the hyperangular and the hyperradius variables and the trace over the spin and isospin degrees of freedom. By using the orthogonality properties of the HH states, Eq. (F.2) reduces to

$$\langle r_\alpha^2 \rangle_p = \frac{1}{12} \sum_{l,l'} \sum_{KLST} \sum_{\alpha, \alpha'} c_{l,\alpha}^{KLST} N_{\alpha, \alpha'}^{KLST1+} c_{l', \alpha'}^{KLST},$$  \hspace{1cm} (F.3)

where $N_{\alpha, \alpha'}^{KLST1+}$ is the norm of the HH states as defined in Eq. (2.58), $c_{l,\alpha}^{KLST}$ are the variational parameters as given in Eq. (2.61), and

$$I_{l,l'} = \int_0^\infty d\rho \rho^{14} f_l(\rho) \rho^2 f_{l'}(\rho),$$  \hspace{1cm} (F.4)

where functions $f_l(\rho)$ are defined in Eq. (2.62).

F.2 Magnetic dipole moment

The calculation of the magnetic dipole moment can be easily performed through the use of the auxiliary operator $\hat{S}_z$ and $\hat{L}_z$ defined in Eqs. (3.31) and (3.32) respectively. In fact, the $^6$Li wave function can be easily rewritten in term of its $L$ and $S$
components $\Psi_{LM,SM_s}$, namely

$$\Psi_{6Li}(J_z = +1) = \sum_{L,S M_s} \sum_{M,M_s} (LM, SM_s|11) \Psi_{LM,SM_s}.$$  \hspace{1cm} (F.5)

By computing now the mean value of $\hat{S}_z$ and $\hat{L}_z$, we obtain

$$\langle S_z \rangle = \sum_{L,S M_s} \sum_{M,M_s} M_s (LM, SM_s|11)^2 P_{LS},$$  \hspace{1cm} (F.6)

and

$$\langle L_z \rangle = \sum_{L,S M_s} \sum_{M,M_s} M (LM, SM_s|11)^2 P_{LS},$$  \hspace{1cm} (F.7)

where $P_{LS}$ is the percentage of the $2S+1L$ component in the $^6\text{Li}$ wave function, which is defined as

$$P_{LS} = \langle \Psi_{LM,SM_s}|\Psi_{LM,SM_s} \rangle.$$  \hspace{1cm} (F.8)

### F.3 Electric quadrupole moment

The calculation of the electric quadrupole moment is performed by using the auxiliary operator $\hat{Q}(6)$ defined in Eq. (3.40), so that

$$\langle Q \rangle = \langle \Psi_{6Li}|\hat{Q}(6)|\Psi_{6Li} \rangle_{\Omega,\rho}.$$  \hspace{1cm} (F.9)

As already discussed in Section 3.3.2, the calculation of this operator is much simplified by using the $Q$ hyperangular variables defined in Eq. (3.42). Therefore, we obtain which gives

$$\langle Q \rangle = 2\sqrt{5\pi} |\Psi^Q_{6Li}| \rho^2 \cos \varphi^Q_5 Y_{20}(\hat{x}^Q_5)|\Psi^Q_{6Li} \rangle_{Q^2,\rho},$$  \hspace{1cm} (F.10)

where $\Psi^Q_{6Li}$ is the $^6\text{Li}$ wave function expressed in terms of the new set of variables “$Q$” and the integration is performed over the hyperangular variables $Q^2$. This change of variables represents an orthonormal rotation in the coordinate space. Therefore the independent states, with which we write the $^6\text{Li}$ wave function in the “standard” set of coordinate, will remain independent without changing the expansion of the wave function and the value of the variational parameters. We can rewrite the HH states of Eq. (2.47) as

$$\Psi^K_{\alpha LSTJ\pi}(\Omega_5) = \sum_{\alpha'} A^K_{\alpha\alpha',Q} \Phi^K_{\alpha LSTJ\pi}(\Omega_5),$$  \hspace{1cm} (F.11)

where $A^K_{\alpha\alpha',Q}$ are new TC which permits to rewrite the HH antisymmetrized states constructed using the “standard” set of hyperangular variables in terms of the HH states build with the “$Q$” set. The calculation of these is discussed in Appendix B. The functions $\Phi^K_{\alpha LSTJ\pi}(\Omega_5^Q)$ are the one defined in Eq. (2.49) written in term of the “$Q$” variables. In such a way, Eq. (3.39) can be rewritten as

$$\langle Q \rangle = 2\sqrt{5\pi} \sum_{\xi,\xi'} \varepsilon_{\xi} \varepsilon'_{\xi'} \sum_{\mu,\mu'} A^K_{\alpha \mu,\xi} A^{K' L'S'T' J\pi, Q} \times \langle f_l(\rho)\Phi^K_{\alpha' LSTJ\pi} | \rho^2 \cos \varphi_5^Q Y_{20}(\hat{x}^Q_5) | f_l^\prime(\rho)\Phi^K_{\alpha' LSTJ\pi} \rangle_{Q^2,\rho},$$  \hspace{1cm} (F.12)
Appendix F. Details of the calculation of \(^6\)Li electromagnetic static properties

where \(\xi \equiv \{KLST\alpha\}\). Thanks to the use of the “Q”-variables this integral, can be
easily factorized in pieces, obtaining

\[
\langle f_l(\rho)|\rho^2|f'_l(\rho)\rangle = \langle f_l(\rho)|\rho^2|f'_l(\rho)\rangle_{\Omega\Omega},
\]

where the integrals \(\langle f_l(\rho)|\rho^2|f'_l(\rho)\rangle_{\Omega}\) as given in Eq. (F.4), and

\[
\langle \Phi_{KLST J\pi}^\alpha|\cos \phi_{Q5}^2 Y_{20}(\hat{x}_5^Q)\rangle =
C_{LL'SJ}^{\ell_5,\ell'_5,4} \prod_{i=2}^4 \delta_{\ell_i,\ell'_i} \delta_L \delta_{n_i,n'_i} \prod_{i=2}^6 \delta_{S_i,S'_i} \delta_{T_i,T'_i} \delta_{TT'},
\]

with

\[
C_{LL'SJ}^{\ell_5,\ell'_5,4} = \sqrt{\frac{3}{8\pi}} (-1)^{1+L_4+S} \frac{2 L_4 L'_4}{2} \left\{ \begin{array}{c} 2 \ 2 \\ L \\ L' \end{array} \right\} \left\{ \begin{array}{c} 2 \ 2 \\ \ell_5 \\ \ell'_5 \\ \ell_5 \\ \ell'_5 \end{array} \right\} \left( \begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{array} \right),
\]

and

\[
I(K_4, \ell_3 n_5, \ell'_3 n'_5) = \frac{N_{n_5}^{\ell_5} N_{n'_5}^{\ell'_5}}{2^8 \sqrt{2}} \times \int_1^{-1} dy \left( 1 + y \right)^{\ell_5+\ell'_5+3} \left( 1 - y \right)^{K_4+5} P_{n_5}^{\ell_5,\ell_5+1/2}(y) P_{n'_5}^{\ell'_5,\ell'_5+1/2}(y).
\]

The integrals in Eq. (F.4) and (F.16) can be calculated using the Gauss integrations
technique in an essentially exact way (only limited by the internal numerical accu-
rracy of the computer system). Therefore, the only approximation of the computation
of the quadrupole moment is related to the accuracy of the wave function.

The use of the “Q” variables permits to reduce drastically the number of coupling
between the states. In fact, all the quantum number that describe a states
except for \(l, \ell_5, n_5, L\), are constrained by Kronecker’s \(\delta\)-functions. In such a way,
also the computational time required is quite reduced. In order to test the change of
variables, we computed also the quadrupole moment by using the standard hyper-
spherical angle variables for the first values of \(K\), obtaining exactly the same value
calculated using the \(Q\) variables.
Appendix G

Calculation of the $\alpha + d$ cluster form factor

In this appendix we derive the explicit expression of the $\alpha + d$ CFF defined in Eq. (4.15) in term of the HH functions. We start from Eq. (4.18), which is written using the Jacobi coordinates of the set “B”. This appendix is organized as follows. In the first section we rewrite the $^6$Li, $\alpha$ and $d$ wave functions in terms of the Jacobi coordinates “B”. In the second section we derive the explicit form of the CFF in term of the HH functions.

G.1 The wave function in term of the set “B”

To compute the integral of Eq. (4.18) we need to express the wave function of $^6$Li as given in Eq. (2.61) in term of the Jacobi coordinates of set “B” given in Eq. (2.5). We define the hyperangles relative to the set “B” as

$$
\cos \varphi_{2B} = \frac{x_{4B}}{\sqrt{x_{3B}^2 + x_{4B}^2}}, \\
\cos \varphi_{3B} = \frac{x_{5B}}{\sqrt{x_{3B}^2 + x_{4B}^2 + x_{5B}^2}}, \\
\cos \varphi_{4B} = \frac{x_{1B}}{\sqrt{x_{3B}^2 + x_{4B}^2 + x_{5B}^2 + x_{1B}^2}}, \\
\cos \varphi_{5B} = \frac{x_{2B}}{\sqrt{x_{3B}^2 + x_{4B}^2 + x_{5B}^2 + x_{1B}^2 + x_{2B}^2}}.
$$

(G.1)

Note the definition of $\varphi_{2B}$ and $\varphi_{3B}$. In this way they are identical to the $A = 4$ hyperangles used to construct the wave function of the $\alpha$ particle. The corresponding six-body HH functions are

$$
Y_{\mu}^{KLM}(\Omega_B) = \left( \left( (Y_{\ell_1}(\hat{x}_{1B})Y_{\ell_2}(\hat{x}_{2B}))_{L_2} Y_{\ell_3}(\hat{x}_{3B}) \right)_{L_3} Y_{\ell_4}(\hat{x}_{4B}) \right)_{L_4} Y_{\ell_5}(\hat{x}_{5B}) \right)_{LM} \times P_{n_2,n_3,n_4,n_5}^{\ell_3,\ell_4,\ell_5,\ell_1,\ell_2}(\varphi_{2B}, \varphi_{3B}, \varphi_{4B}, \varphi_{5B}),
$$

(G.2)
where
\[
\mathcal{P}_{n_2,n_3,n_4,n_5}^{\ell_3,\ell_4,\ell_5,\ell_1,\ell_2} (\varphi_{2B}, \varphi_{3B}, \varphi_{4B}, \varphi_{5B}) = \\
N_{n_2}^{\ell_3,\ell_4} (\cos \varphi_{2B}) N_{n_3}^{\ell_5,\ell_1} (\sin \varphi_{3B}) N_{n_4}^{\ell_2,\ell_5} (\cos 2 \varphi_{3B}) \times K_1 \times K_2 \times K_3 \times K_4, \tag{G.3}
\]
while
\[
K_1 = \ell_3, \\
K_2 = \ell_3 + \ell_4 + 2n_2, \\
K_3 = \ell_3 + \ell_4 + \ell_5 + 2n_2 + 2n_3, \\
K_4 = \ell_3 + \ell_4 + \ell_5 + \ell_1 + 2n_2 + 2n_3 + 2n_4 + 2n_5, \\
\]
and
\[
\nu_1 = \ell_3 + \frac{1}{2}, \\
\nu_2 = \ell_3 + \ell_4 + 2n_2 + 2, \\
\nu_3 = \ell_3 + \ell_4 + \ell_5 + 2n_2 + 2n_3 + \frac{7}{2}, \tag{G.4}
\]
\[
\nu_4 = \ell_3 + \ell_4 + \ell_5 + \ell_1 + 2n_2 + 2n_3 + 2n_4 + 5, \\
\nu_5 = \ell_3 + \ell_4 + \ell_5 + \ell_1 + \ell_2 + 2n_2 + 2n_3 + 2n_4 + 2n_5 + \frac{13}{2}. \tag{G.5}
\]

This particular choice of the hyperangular coordinates and definition of the HH function is different compared to the standard Zernike and Brinkman representation [67,68] but it is very advantageous when we will compute the overlap as it will be clear in the following.

We need now to find a way to express the HH functions of Eq. (2.44), written in terms of the standard coordinates, in terms of those defined in Eq. (G.2), written with set “B” of coordinates. This transformation is performed by using new TC $A_{\beta,\beta'}^{K_{L_5}S_6T_6B}$ (see Appendix B for the details), with which we can rewrite the wave function of $^6$Li as

\[
\Psi_{6Li} = \sum_{K_{L_5}S_6T_6} \sum_{\beta,\beta'} A_{\beta,\beta'}^{K_{L_5}S_6T_6B} f_1(\rho) A_{\beta,\beta'}^{K_{L_5}S_6T_6B} \mathcal{P}_{n_2,n_3,n_4,n_5}^{\ell_3,\ell_4,\ell_5,\ell_1,\ell_2} (\varphi_{2B}, \varphi_{3B}, \varphi_{4B}, \varphi_{5B}) \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \times \time
coordinates, we have

\[ \Psi_d(x_{1B}) = \sum_{\ell_d=0,2} u_{\ell_d}(x_{1B}) \left[ Y_{\ell_d}(\hat{x}_{1B}) (\sigma_5 \sigma_6) S_d \right] J_d L_{\alpha_d} (\tau_5 \tau_6) T_d T_{\alpha_d}, \tag{G.7} \]

where \( J_d = 1, S_d = 1 \) and \( T_d = 0 \) and the \( u_{\ell_d}(x_{1B}) \) functions are determined solving the Schrödinger equation for the deuteron. The wave function of the \( \alpha \) particle depends on the coordinates of particles \((1, 2, 3, 4)\). Written using the Jacobi coordinates “B” \( x_{3B}, x_{4B} \) and \( x_{5B} \), it reads

\[ \Psi_\alpha(x_{3B}, x_{4B}, x_{5B}) = \sum_{K_\alpha} \sum_{L_\alpha} K_{\alpha} L_{\alpha} S_{\alpha} T_{\alpha} f_{\alpha}(\rho_4) \sum_{\beta_\alpha, \ell_\alpha} A_{\beta_\alpha, \ell_\alpha} \left( (\tau_1 \tau_2) T_{\alpha_d} (\tau_3), \tau_4 \right) T_{\alpha_d}, \tag{G.8} \]

where \( J_\alpha = 0, \rho_4 = \sqrt{x_{3B}^2 + x_{4B}^2 + x_{5B}^2} \), \( A_{\beta_\alpha, \ell_\alpha} \) are the TC for the four-body system,

\[ f_{\alpha}(\rho_4) = \frac{2}{\gamma_\alpha} \sqrt{\frac{1!}{(l_\alpha + 8)!}} \frac{L_{(l_\alpha)}(\gamma_\alpha \rho_4) e^{-\frac{\rho_4^2}{2}}}{(\gamma_\alpha \rho_4)} \tag{G.9} \]

\[ \beta_\alpha \equiv \{ \ell_1, \ell_2, \ell_3, L_2, n_2, n_3, S_2, S_3, T_2, T_3 \} \tag{G.10} \]

and

\[ P_{n_2, n_3}^{\ell_1, \ell_2, \ell_3} (\varphi_{2B}, \varphi_{3B}) = \lambda_{n_2, n_3}^{\ell_1, \ell_2, \ell_3} (\cos \varphi_{2B})^{\ell_2} (\sin \varphi_{2B})^{\ell_3} P_{n_2, n_3}^{\ell_1 + 1/2, \ell_2 + 1/2} (\cos 2\varphi_{2B}) \]

\[ \times \lambda_{n_2, n_3}^{\ell_1, \ell_2, \ell_3} (\cos \varphi_{3B})^{\ell_3} (\sin \varphi_{3B})^{\ell_3} (n_2, n_3) K_{\alpha} P_{n_2, n_3}^{\ell_1, \ell_2, \ell_3} (2 \cos 2\varphi_{3B}), \tag{G.11} \]

We remark again that the coordinates \( x_{3B}, x_{4B}, x_{5B} \) and hyperangles \( \varphi_{2B}, \varphi_{3B} \) correspond exactly to the standard Jacobi coordinate and hyperangles we use to compute the \( \alpha \) wave function. Therefore no transformation of the four-body HH states is needed in this case.

### G.2 Explicit calculation of the overlap integral

By using the form of the wave functions discussed in the previous Section, it is now possible to compute the integral of Eq. (4.18). In this section we will drop the “B” index on the Jacobi and hyperangular variables, since we will consider only these variables. Moreover, also the quantum numbers \( \nu_i \) and \( K_i \) which will appear in this Section are the ones defined in Eqs. (G.4) and (G.5), respectively.

The isospin term of the \( \psi_{\alpha+d} \) wave function can be rewritten as

\[ \left[ \left( \tau_1 \tau_2 \right) T_{3a} (\tau_3) T_{3a} (\tau_4) \right] T_{3a}, T_{\alpha_d}, \left( \tau_5 \tau_6 \right) T_{\alpha_d} T_{\alpha_d} \tag{G.12} \]

\[ = \sum_t C(T_{3a}, t) \left[ \left( \tau_1 \tau_2 \right) T_{3a} (\tau_3) T_{3a} (\tau_4 \tau_5) T_{3a} (1/2) \right] T_{3a}, T_{\alpha_d}, \tag{G.13} \]

where

\[ C(T_{3a}, t) = (-1)^{2T_{3a} + 1} \frac{\ell}{2}, \tag{G.13} \]
with $i = \sqrt{2i+1}$ and we use the fact that $T_d = 0$. The trace on the isospin in Eq. (4.18) results in

\[
\left[ ((\tau_1\tau_2)T_{2a}\tau_3)T_{3a}\tau_4 \right]^{\dagger} T_{a}^{\dagger} T_{a} = C(T_3, T_4)\delta_{T_{2a}, T_2}\delta_{T_{3a}, T_3}\delta_{T_1, 1/2}\delta_{T_a, T_6}. \tag{G.14}
\]

For the spin part of the cluster wave function, we recouple the angular and spin terms such as

\[
\left\{ \left\{ \left[ ((Y_{\ell_1a}(\hat{x}_3)Y_{\ell_2a}(\hat{x}_4))L_{2a}, Y_{\ell_3a}(\hat{x}_3)) \right]_{L_a} \left[ ((\sigma_1\sigma_2)S_{2a}, \sigma_3)S_{3a}, \sigma_4 \right]_{S_a} \right\}_0 \right. 
\times [Y_{\ell_d}(\hat{x}_1)(\sigma_5\sigma_6)S_d]_1 \left. \right\}_{J J_s} 
= \sum_{L_{a}^dL_{a}^{\dagger}\ell_{2a}^{\dagger}S_{2a}^{\dagger}\ell_{3a}^{\dagger}S_{3a}^{\dagger}} A_{L_{3a}S_{3a}J_{a}J_{d}}^L S_{a}^{\dagger} S_{d}^{\dagger} A_{L_{2a}S_{2a}J_{a}J_{d}}^{L_{d}} S_{a}^{\dagger} S_{d}^{\dagger} Y_{\ell_1a}(\hat{x}_3) Y_{\ell_2a}(\hat{x}_4) Y_{\ell_3a}(\hat{x}_5) \right\}_{L_{5}}, \tag{G.15}
\]

where

\[
A_{S_{3a}S_{3a}J_{a}J_{d}}^{L_{d}L_{1a}L_{2a}L_{3a}L_{a}} (L_{2}^{d}L_{a}^{d}L_{d}^{d}S_{d}^{d}S_{d}^{d}S_{d}^{d}) = (-1)^{1+L+L_{1a}+L_{2a}+L_{3a}+L_{a}+L_{2a}+L_{4}+S_{3a}+S_{4}+S_{6}} \times 3 \hat{\ell}_{d}^{d} \hat{L}_{b}^{d} \hat{L}_{d}^{d} \hat{\ell}_{1b}^{d} \hat{\ell}_{2b}^{d} \hat{\ell}_{3b}^{d} \hat{\ell}_{a}^{d} \hat{\ell}_{2a} \hat{S}_{a} \begin{pmatrix} L_{a} & S_{a}^{d} & 0 \\
L_{2a} & 1 & J \\
L_{5a} & S_{5}^{d} & J \end{pmatrix} \begin{pmatrix} L & L_{d}^{d} \end{pmatrix} \begin{pmatrix} \ell_{1a} & 1/2 & S_{a}^{d} \\
\ell_{2a} & 1/2 & S_{4}^{d} \end{pmatrix} \begin{pmatrix} \ell_{3a} & 1/2 & S_{5}^{d} \\
\ell_{4a} & 1/2 & S_{6}^{d} \end{pmatrix} \begin{pmatrix} S_{3a} & 1/2 & S_{a}^{d} \\
S_{4a} & 1/2 & S_{4}^{d} \end{pmatrix}. \tag{G.16}
\]

It is now possible to compute the integrals over the angular variables $\hat{x}_a$ and the trace on the spins

\[
\int \left( \prod_{\lambda=1}^{5} d\hat{x}_{\lambda} \right) \left\{ \left[ ((Y_{\ell_1a}(\hat{x}_3)Y_{\ell_2a}(\hat{x}_4))L_{2a}, Y_{\ell_3a}(\hat{x}_3)) \right]_{L_a} \left[ ((\sigma_1\sigma_2)S_{2a}, \sigma_3)S_{3a}, \sigma_4 \right]_{S_a} \right\}_0 \right. 
\times Y_{\ell_1}(\hat{x}_1)(\sigma_5\sigma_6)S_1 \right\}_{J J_s} 
\times \left\{ \left[ ((Y_{\ell_1}(\hat{x}_1)Y_{\ell_2}(\hat{x}_2))L_2 Y_{\ell_3}(\hat{x}_3) \right)_{L_3} Y_{\ell_4}(\hat{x}_4) Y_{\ell_5}(\hat{x}_5) \right\}_{L_5} 
\times \left[ ((\sigma_1\sigma_2)S_{2a}S_{3a}, (\sigma_4\sigma_5)S_{4a}S_{6a}) \right]_{S_6} \right\}_{J_a J_{a}} = A_{S_{3a}S_{3a}J_{a}J_{d}}^{L_{d}L_{1a}L_{2a}L_{3a}L_{a}} (L_{2}^{d}L_{a}^{d}L_{d}^{d}S_{d}^{d}S_{d}^{d}S_{d}^{d}) \times \delta_{\ell_{1a}^{d}\ell_{2a}^{d}\ell_{3a}^{d}L_{a}^{d}} \delta_{\ell_{4a}^{d}\ell_{5a}^{d}} \delta_{\ell_{2a}^{d}\ell_{3a}^{d}} \delta_{S_{2a}^{d}S_{3a}^{d}S_{4a}^{d}S_{5a}^{d}S_{6a}^{d}} \delta_{J_{a}^{d}J_{a}^{d}J_{a}^{d}}. \tag{G.17}
\]
We can now use these results to rewrite Eq. (4.18) as

\[
\frac{f_L(r)}{r} = \sqrt{15} \left( \frac{\sqrt{6}}{4} \right)^{\frac{3}{2}} \sum_{K_a L_a S_n T_{\alpha} \beta} \sum_{\beta, \ell} \sum_{\beta, \ell} \sum_{\beta, \ell} a_{\beta, \alpha, \beta, \ell} A_{\beta, \ell}^{K_a L_a S_n T_{\alpha},(4)} \int \left( \prod_{i=1}^{5} dx_i x_i^2 \right) \times \delta \left( \frac{3}{8} x_2 - r \right) f_{\alpha}(\rho_4) f_i(\rho) \sum_{\ell_d} u_{\ell_d}(x_1) \sum_{\tilde{\beta} \tilde{\alpha}, \tilde{\beta} \tilde{\alpha}} A_{\tilde{\beta} \tilde{\alpha}, \tilde{\beta} \tilde{\alpha}, \ell_d}^{K_a L_a S_n T_{\alpha},(4)} \int \left( \prod_{i=1}^{5} dx_i x_i^2 \right) \times P_{\ell_3, \ell_4, \ell_5, \ell_6, \ell_7}^{\tilde{\ell}_3, \tilde{\ell}_4, \tilde{\ell}_5, \tilde{\ell}_6, \tilde{\ell}_7} (\varphi_2, \varphi_3) P_{\ell_3, \ell_4, \ell_5, \ell_6, \ell_7}^{\tilde{\ell}_3, \tilde{\ell}_4, \tilde{\ell}_5, \tilde{\ell}_6, \tilde{\ell}_7} (\varphi_2, \varphi_3, \varphi_4, \varphi_5) \times A_{\tilde{\beta} \tilde{\alpha}}^{\ell_3, \ell_4, \ell_5, \ell_6} (L_2 L_3 L_4 L_5 S_4 S_5 S_6) C(T_3, T_4) \delta_{\tilde{\beta} \tilde{\alpha}, \tilde{\beta} \tilde{\alpha}, \ell_d} \delta_{\tilde{\beta} \tilde{\alpha}, \ell_d} \delta_{\tilde{\beta} \tilde{\alpha}, \ell_d} L, \tag{G.18}
\]

where

\[
\tilde{\beta} \tilde{\alpha} \equiv \{ \ell_3, \ell_4, \ell_5, S_2', T_2', T_3', T_4', T_6' \} \tag{G.19}
\]

and

\[
\tilde{\beta} \tilde{\alpha} \equiv \{ \ell_1, \ell_2', \ell_3, S_2', T_2', T_3', T_4', T_6', 1/2, T_4' \} \tag{G.20}
\]

We can now rewrite the integral variables as

\[
\int \left( \prod_{i=1}^{5} dx_i x_i^2 \right) = \int_0^\infty dx_2 x_2^2 \int_0^\infty d\rho_5 \rho_5^{11} \int_0^\pi d\varphi_1 \cos^2 \varphi_1 \sin^{3-4} \varphi_i \tag{G.21}
\]

In this way, thanks to the definition of the \( \varphi_i \) angles in Eq. (G.1), the integrals on \( d\varphi_2 \) and \( d\varphi_3 \) are reduced by using the orthonormal properties of the Jacobi polynomials, i.e.

\[
\int_0^\pi \left( \prod_{i=2,3} d\varphi_i \cos^2 \varphi_i \sin^{3-4} \varphi_i \right) P_{n_{2,3}}^{\ell_3, \ell_4, \ell_5} (\varphi_2, \varphi_3) P_{n_{2,3}}^{\ell_3, \ell_4, \ell_5} (\varphi_2, \varphi_3, \varphi_4, \varphi_5) = \delta_{n_{2,3}, n_{2,3}} \Lambda_{n_{2,3}}^{\ell_3, \ell_4, \ell_5} (\cos \varphi_2 \varphi_3) K_{n_{2,3}}^{\ell_3, \ell_4, \ell_5} (\sin \varphi_2 \varphi_3) K_{n_{2,3}, n_{2,3}}^{\ell_3, \ell_4, \ell_5} \left( \cos \varphi_2 \varphi_3 \right) \tag{G.22}
\]

The variables \( \rho_4 \) and \( x_1 \) explicitly depend on \( \varphi_4 \). In fact, by using Eq. (G.1) and the definition of \( \rho_4 \), we have \( \cos \varphi_4 = x_1 / \sqrt{\rho_4^2 + x_1^2} \), and therefore \( \rho_4 = \rho_5 \sin \varphi_4 \) and \( x_1 = \rho_5 \cos \varphi_4 \). Therefore the integral on \( \varphi_4 \) reads

\[
I_{\ell_d, \alpha}^{K_3, \ell_1, n_4} (\rho_5) = \Lambda_{n_4}^{\ell_1, \ell_4} \int_0^\pi d\varphi_4 (\cos \varphi_4)^{2+\ell_1} (\sin \varphi_4)^{8+K_3} \times f_{\alpha} (\rho_5 \sin \varphi_4) \sum_{\ell_d} (\rho_5 \cos \varphi_4) P_{n_4}^{\ell_4, \ell_4, \ell_4+1} (\cos 2\varphi_4), \tag{G.23}
\]

which can be evaluated using the Gauss-Techebychev quadrature. What remains to be calculated is the integration over \( \rho_5 \) which explicitly reduce to

\[
I_{\ell_d, \alpha}^{K_3, \ell_1, n_4, \ell_2, n_5} (r) = \Lambda_{n_5}^{\ell_2, \ell_2} \int_0^\infty d\rho_5 \rho_5^{11} I_{\ell_d, \alpha}^{K_3, \ell_1, n_4} (\rho_5) f_1 (\sqrt{\rho_5^2 + 8/3 r^2}) \times \left( \frac{\sqrt{8/3 r}}{\sqrt{\rho_5^2 + 8/3 r^2}} \right)^{\ell_2} \left( \frac{\rho_5}{\sqrt{\rho_5^2 + 8/3 r^2}} \right)^{K_4} P_{n_5}^{\ell_2, \ell_2+1/2} \left( \frac{8/3 r^2 - \rho_5^2}{\rho_5^2 + 8/3 r^2} \right). \tag{G.24}
\]

Also in this case the integral can be computed using Gauss-Legendre quadrature.
The final expression for the CFF is then obtained by eliminating the integral on \( x_2 \) through the \( \delta \)-function and it reads

\[
\frac{f_L(r)}{r} = \sqrt{15} \left( \frac{2\sqrt{2}}{\sqrt{3}} \right)^{\frac{3}{2}} r^2 \sum_{L_\alpha, S_\alpha, T_\alpha} \sum_{L_\beta, S_\beta, T_\beta} \sum_{\ell_a, \ell_b} \sum_{\ell_c, \ell_d} a_{L_\alpha, S_\alpha, T_\alpha, L_\beta, S_\beta, T_\beta, \ell_a, \ell_b} \times \\
\times \sum_{\ell_c, \ell_d} A_{L_\alpha, S_\alpha, T_\alpha, L_\beta, S_\beta, T_\beta, \ell_c, \ell_d} \times \sum_{\ell_a, \ell_b} A_{L_\alpha, S_\alpha, T_\alpha, L_\beta, S_\beta, T_\beta, \ell_a, \ell_b} \times \\
\times C(T_3', T_4') \times \delta_{\ell_a, \ell_c} \delta_{\ell_b, \ell_d} \delta_{\ell_3, \ell_4} \delta_{n_2, n_3} \delta_{n_3, n_5} \delta_{\ell_1, \ell_2} \delta_{\ell_5, \ell_6} \delta_{n_4, n_5} \delta_{n_5, n_6}.
\] (G.25)

Some final comments are needed before concluding. The use of the variables “B” increases drastically the precision of the overlap calculation. In fact, by passing from the “standard” set to the “B” set, the dimension of the integrals to be computed diminishes from five to two, decreasing the numerical errors. The final accuracy in the calculation of these integrals depends on the number of Chebyshev and Legendre points that we use. For the calculation of these integrals, we used up to 300 points obtaining a precision of the order of \( 10^{-7} \) – \( 10^{-8} \). We note that the integrals involve functions with exponential tail multiplied by Jacobi polynomials, having an oscillating behavior. The accuracy reached is in any case sufficient to have stable results for the ANCs.
Appendix H

Calculation of the coefficients $c_{\frac{KLST}{L,\beta}}(\xi)$

The coefficients $c_{\frac{KLST}{L,\beta}}(\xi)$ given in Eq. (4.44) can be evaluated by using the orthonormality properties of the HH basis, i.e.

$$c_{\frac{KLST}{L,\beta}}(\xi) = \langle \Phi_{\frac{KLST}{L,\beta}}(p=1) | \Psi_{LSJ}^{\alpha+d}(p=1) \rangle \Omega_{B,\rho},$$  \hspace{1cm} (H.1)

where $\langle \cdots | \cdots \rangle_{\Omega_{B,\rho}}$ represents the integration over all the hypercoordinates and the trace over spin and isospin [see Eq. (4.45)].

As regarding the trace over the isospin, it is easy to show that we obtain exactly the result given in Eq. (G.14). Also for the integration over the variables $\hat{x}_i B$ and the spin trace the result is equal to the one given in Eq. (G.17). By using these results and the orthonormality properties of the Jacobi polynomials as discussed in Eq. (G.22), Eq. (4.45) reduces to

$$c_{\frac{KLST}{L,\beta}}(\xi) = \int_0^{\infty} d\rho \rho^{14} f_\rho^{KLST}(\rho, \xi),$$  \hspace{1cm} (H.2)

where

$$f_\rho^{KLST}(\rho, \xi) = \sum_{\ell_4} \sum_{\beta_4, \alpha_4} a_{\beta_4, \alpha_4} \frac{\tilde{\beta}_4}{L_4^{\ell_4}}(\rho, \xi)$$

$$\times A_{S_{5a}, S_{5a}}(L_2 L_4 L_5 S_3 S_3) \delta_{\tilde{\ell}_4, \ell_4} \tilde{T}_4, \tilde{T}_3, \tilde{T}_2, \tilde{T}_1, \tilde{T}_0 C(\tilde{T}_3, \tilde{T}_4).$$  \hspace{1cm} (H.3)

Here we have defined

$$\tilde{\beta}_4 = \{ \ell_1, \ell_2, \ell_3, \alpha_4, T_2, T_3, T_4, 1/2, T_5 \},$$  \hspace{1cm} (H.4)

and

$$\bar{\beta}_4 = \{ \ell_3, \ell_4, S_2, S_3, T_2, T_3, T_5, T_6 \}.$$  \hspace{1cm} (H.5)

Moreover, $\tilde{\beta}$ is the complete set of quantum numbers which describe a six-body quantum state as defined in Eq. (2.50), and $a_{\beta_4, \alpha_4}$ are the variational parameter of the $\alpha$-particle wave function computed by solving the four-body problem [see
Appendix H. Calculation of the coefficients $c_{LST}(\xi)$

Eq. (4.4)]. The function $I_{Ld_{d\alpha}}^K_{\ell_1\bar{n}_4\ell_2\bar{n}_5}(\rho, \xi)$ is given by

$$I_{Ld_{d\alpha}}^K_{\ell_1\bar{n}_4\ell_2\bar{n}_5}(\rho, \xi) = 2^{\ell_2+\ell_3+15}N_{\bar{n}_5}e_{\ell_2,\ell_5} \int_{-1}^{1} dy(1+y)^{\ell_2+1}/(1-y)^{\ell_3+10}F_{\bar{n}_5}^\rho \ell_2+1/2(y)$$

$$\times F \left( \sqrt{\frac{3}{8}} \sqrt{\frac{1+y}{2}}, \xi \right) I_{\ell_1\bar{n}_4}(y, \rho) , \quad \text{(H.6)}$$

where

$$I_{\ell_1\bar{n}_4}(y, \rho) = 2^{\ell_1+\ell_3+12}N_{\bar{n}_4}e_{\ell_1,\ell_4} \int_{-1}^{1} dx(1+x)^{\ell_1+1}/(1-x)^{\ell_3+7}F_{\bar{n}_4}^\rho \ell_1+1/2(x)$$

$$\times u_{\ell_1d} \left( \rho \sqrt{\frac{1-y}{2}} \sqrt{\frac{1+x}{2}} \right) \tilde{f}_{\bar{n}_4} \left( \rho \sqrt{\frac{1-y}{2}} \sqrt{\frac{1-x}{2}} \right) , \quad \text{(H.7)}$$

and $F$ is a generic intercluster function which can depend on additional quantum number $\xi$. The integrals of Eqs. (H.6) and (H.7) are computed using the Gauss-Tchebychev quadrature. In order to obtain an accuracy of $\sim 10^{-7} - 10^{-8}$ for values of $\rho$ between 0 and 10 fm, we need to use 300 points for the integration. We do not notice any significant improvement in the precision by using a larger number of integration points. Moreover, we notice that the accuracy decreases rapidly when $\rho > 10$ fm. The integral in Eq. (H.2) is then computed by using an exact Lagrange-Gauss quadrature formula, with no lose of accuracy.
Appendix I

Derivation of the cross section and angular distribution expressions for $A_1 + A_2 \rightarrow A_3 + \gamma$

In this appendix we explicitly derive the formulas for the total cross section, given in Eq. (5.4), and the angular distribution of the emitted photon, given in Eq. (5.12).

Let us consider the generic reaction $A_1 + A_2 \rightarrow A_3 + \gamma$ where $A_1$ has total angular momentum $J_1, M_1$ and so on, while with $\lambda$ we indicate the polarization of the photon. By using the Fermi Golden rule it is easy to derive the explicit expression of the differential cross section by evaluating the phase space, namely

$$
\frac{d\sigma_{J_3}}{d\Omega_q} = \frac{e^2}{8\pi v_{\text{rel}} 1 + q/m_3 (2J_1 + 1)(2J_2 + 1)} \sum_{M_1, M_2} \sum_{M_3, \lambda} |M_{J_1, M_2, M_3, \lambda}(q)|^2,
$$

where $v_{\text{rel}}$ is the relative velocity of the two incoming particles, $q$ is the photon momentum and $m_3$ is the mass of $A_3$ nucleus. The matrix element $M_{J_1, M_2, M_3, \lambda}(q)$ is given by

$$
M_{J_1, M_2, M_3, \lambda}(q) = \hat{p} \langle J_3 M_3 | H_I(\lambda, q) | J_1 M_1, J_2 M_2 \rangle \hat{p}
$$

where $|J_1 M_1, J_2 M_2 \rangle$ and $|J_3 M_3 \rangle$ are the wave functions of the scattering and the bound state as defined in Eqs. (5.1) and (5.3), respectively (quantized along the $\hat{p}$ axis, where $\hat{p}$ is the momentum of the incident particles) and $H_I$ is the interaction Hamiltonian given by

$$
H_I(\lambda, q) = \sum_{\Lambda \geq 1} (-i)^\Lambda (2\Lambda + 1) [E_{\Lambda, -\lambda}(q) + \lambda M_{\Lambda, -\lambda}(q)].
$$

The above expression is valid in the frame where $q$ is along $z$ and $E_{\Lambda, -\lambda}(M_{\Lambda, -\lambda})$ are the electric (magnetic) operator multipole as defined in Ref. [100]. We have now to remember that the photon is emitted in an arbitrary direction, while our states are quantized along the direction of the incoming momentum. Because in the experiment we are measuring the photon and consequently its direction, we need to rotate our nuclear state of a $\theta$ angle in order to report it on the photon direction. Formally this is equivalent to rotate back the photon direction on the $\hat{p}$-axis, which reduces the interaction Hamiltonian in the form

$$
H_I(\lambda, q, \theta) = \sum_{\Lambda \geq 1} \sum_{M} (-i)^\Lambda (2\Lambda + 1) [E_{\Lambda, -\lambda}(q) + \lambda M_{\Lambda, -\lambda}(q)] D_{M, -\lambda}^\Lambda(-\theta),
$$
where $D_{M,-\lambda}^\lambda(-\theta)$ is the rotation matrix. Hence, the matrix element $M_{3J_1, M_2, M_3, \lambda}(q)$ reduces to

$$
|M_{3J_1, M_2, M_3, \lambda}(q)|^2 = \frac{1}{J_1 J_2 J_3} \sum_{LSJ_3 \Lambda M} \sum_{L'SJ_3' \Lambda M'} \hat{L}
\hat{L}' \hat{\Lambda} \hat{\Lambda}'(-i)^{\Lambda - \Lambda' + L' - L}
\times (J_1 M_1, J_2 M_2 | S J_3)(J_1 M_1, J_2 M_2 | S' J_3') (S J_3, L0 | J J_3)(S' J_3', L0 | J' J_3')
\times (J J_3, \Lambda M | J_3 M_3)(J' J_3', \Lambda' M' | J_3 M_3) D_{M,-\lambda}^\lambda(-\theta) D_{M,-\lambda}^{\Lambda \Lambda}(\theta)
\times \left[ E_\lambda^{LSJ_3}(q) + \lambda M_{LSJ_3}(q) \right]^* \left[ E_{\lambda'}^{L'S'J_3'}(q) + \lambda M_{L'S'J_3}(q) \right]^* ,
$$

where $\hat{j} = \sqrt{2J + 1}$ we used the form of the wave functions given in Eqs. (5.1) and (5.3) and $E_\lambda^{LSJ_3}(M_{LSJ_3})$ is the reduced electric (magnetic) matrix element, as defined in Eq. (5.5). We now use the following properties

$$
\sum_{M_1 M_2} (J_1 M_1, J_2 M_2 | S J_3)(J_1 M_1, J_2 M_2 | S' J_3') = \delta_{SS'} \delta_{J J'}, \tag{1.6}
$$

$$
D_{M,-\lambda}^\lambda(-\theta) D_{M',-\lambda}^{\Lambda \Lambda}(\theta) = (-)^{M' - L} \sum_k d_{M-M',0}^k (\theta)
\times (\Lambda M, \Lambda' - M' | k M - M')(\Lambda - \lambda, \Lambda' + \lambda | k0), \tag{1.7}
$$

and the fact that due to the $\delta$-function on $J_z, J'_z$ in Eq. (1.6), we get that $M = M'$. Since $M = M'$ we have that

$$
d_{M-M',0}^k (\theta) = P_k(\cos \theta), \tag{1.8}
$$

where $P_k(\cos \theta)$ are the Legendre polynomials. By using these formulas the matrix element reduces to

$$
\sum_{M_1 M_2 M_3 \lambda} |M_{3J_1, M_2, M_3, \lambda}(q)|^2 = \sum_k a_k^{J_3}(q) P_k(\cos \theta), \tag{1.9}
$$

where

$$
a_k^{J_3}(q) = \frac{1}{J_1 J_2 J_3} \sum_{LL'SJ_3 \Lambda M} \sum_{M_1 M_2} \hat{L}
\hat{L}' \hat{\Lambda} \hat{\Lambda}'(-i)^{\Lambda - \Lambda' + L' - L}
\times (S J_3, L0 | J J_3)(S J_3, L0 | J' J_3)(J J_3, \Lambda M | J_3 M_3)(J' J_3, \Lambda' M | J_3 M_3)
\times (\Lambda M, \Lambda' - M' | k0)(\Lambda - \lambda, \Lambda' + \lambda | k0)
\times \left[ E_\lambda^{LSJ_3}(q) + \lambda M_{LSJ_3}(q) \right]^* \left[ E_{\lambda'}^{L'S'J_3'}(q) + \lambda M_{L'S'J_3}(q) \right]^*. \tag{1.10}
$$

It is easy then to bring Eq. (1.10) in the form of Eq. (5.11) by using the relation between the Clebsch-Gordan and the $6j$ coefficients, i.e.

$$
\sum_{m_1 m_2 m_6} (j_1 m_1, j_2 m_2 | j_3 m_3)(j_6 m_6, j_2 m_2 | j_4 m_4)(j_1 m_1, j_5 m_5 | j_6 m_6)
= (-1)^{j_2 + j_3 + j_5 + j_6} (j_3 m_3, j_5 m_5 | j_4 m_4) \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{array} \right\}. \tag{1.11}
$$

Since the matrix element of Eq. (1.9) does not depend on the angle $\phi$ we can integrate Eq. (1.1) on $d\phi$ obtaining Eq. (5.9).
The total cross section can then be computed by integrating Eq. (5.9) in $d(\cos \theta)$, namely

$$\sigma_{J_3}(E) = \int_{-1}^{1} d(\cos \theta) \sigma_0(E) \sum_k a_{J_3}^k(q) P_k(\cos \theta) = \sigma_0(E) a_{J_3}^0(q),$$

(I.12)

where $\sigma_0(E)$ is given in Eq. (5.10) and only the coefficients $a_{J_3}^0(q)$ survives, and is given by

$$a_{J_3}^0(q) = 2 \sum_{LSJ} |E_{\Lambda}^{LSJ,J_3}(q)|^2 + |M_{\Lambda}^{LSJ,J_3}(q)|^2.$$  

(I.13)

Therefore, we reconstruct exactly Eq. (5.4).
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$f_2(r) \text{[fm}^{-1/2}]$ vs. $r$ [fm]

- $K=2$
- $K=4$
- $K=6$
- $K=8$
- $K=10$
- $K=12$
- Whittaker