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STEPŠYS

Application of the algebraic binary cluster model for six nucleon systems in a translationally invariant basis

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Vilniaus Universitetas
Fizinių ir technologijos mokslų centras

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STEPŠYS

Algebrinio dvinarių klasterių modelio taikymai šešių nukleonų sistemoms transliaciškai invariantinėje bazėje

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List of abbreviations

- **NCSM** No core shell mode
- **TMB** Talmi–Moshinsky bracket
- **HOB** Harmonic oscillator bracket
- **SD** Sleiter determinant
- **CM** Center of mass
- **HH** Hyperspherical harmonics
- **HO** Harmonic oscillator
- **RH** Reduced Hamiltonian
- **CFP** Coefficient of fractional parentage
- **OCFP** Orbital fractional parentage coefficient
- **irrep** Irreducible representation
- **YD** Young Diagram
- **SYT** Standard Young Tableaux
- **REC** Angular momentum recoupling coefficient
- **CG** Clebsch-Gordan coefficient
- **4HOB** Harmonic oscillator transformation brackets for four particles
- **5HOB** Harmonic oscillator transformation brackets for five particles

Introduction

The nuclear theory is a rapidly developing field that contains various theoretical approaches for the description of the nuclear systems. The developments of the computational hardware during 90's and 00's, especially in high-performance computing, presented a big hope that a lot of problems in this field can be solved computationally. This partially became the truth. For example, the UNEDF project was a large collaborative effort, that applied high- performance computing methods for the nuclear many-body problem. For example, the calculation of the ^{12}C isotope required the development of the Asynchronous Dynamic Load Balancing (ADLB) library to efficiently perform the load balancing on more than 100000 cores [1]. Advances in the theoretical description of the nuclei allow us to create better computational models that could calculate more precise, bigger, and more complex systems or to do the same faster and with less computational resources. Experimental physics provides us with a pleiades of data about the microscopic world and, sadly, the theory of nuclear physics lags behind.

Systems like pentaquarks [2, 3, 4] or intrinsic components of baryonic nuclei [5, 6], attract a lot of attention from the theoretical point of view [7, 8]. In nuclear physics, great efforts are being made to understand how the nuclear interaction works [9]. This type of work requires the pursuit of new ways to describe the fermionic systems. The standard ab-initio approach in constructing the model Hamiltonian of such systems with the one particle variables in the harmonic oscillator (HO) basis is not satisfactory. The simplicity and convenience of the one-particle HO basis has its price. The wave functions of bound states must be antisymmetric, characterized by good quantum numbers and translationally invariant for

the strongly coupled N-body system of fermionic nature.

The antisymmetrization procedure using the Slater determinants (SD) is convenient and easily implementable. The constructed antisymmetric one-particle basis, created using the SDs must undertake the additional procedures for the elimination of the center of mass (CM) motion. Moreover, the SD basis results in huge matrix dimensions, therefore requiring enormous computational resources. As a consequence, in recent years there is a noticeable renewed interest in the other types of approaches for the nuclear problem: the SU_3 scheme [10], the symplectic no-core configuration interaction framework [11], and so on.

One of the approaches to the nuclear problem is the algebraic translationally invariant approach. We know that the nucleus is a system that is independent from the external fields. Therefore, the use of the intrinsic coordinates is more desirable as the two-body and the three-body interactions depend on the relative coordinates. One of the possible intrinsic coordinate systems is the Jacobi coordinate system [12, 13]. The advantages of the transition to the Jacobi coordinate system include the explicit elimination of the c.m. motion and the conservation of the good quantum numbers $J^\pi T$ (total angular momentum, parity, and total isospin). This can be done in the coupled HO basis and therefore a significant reduction of the matrix dimensions can be achieved [14]. The Jacobi coordinate basis is used quite often in the No Core Shell Model (NCSM) [15] ab-initio description of nuclei. These coordinates are primarily used for the few-body systems, involving no more than three Jacobi coordinates. In conjunction with the SD basis, the Jacobi coordinates are used for systems larger than four nucleons [15]. In this approach, the antisymmetric wavefunctions are constructed for the subclusters of the system and then the Jacobi coordinates are used to couple the antisymmetrized subclusters.

Another popular approach is to employ Hyperspherical Harmonics (HH). In the HH community often the transition to the hyperspherical coordinates is done from the Jacobi coordinates. Nevertheless, this requires complicated calculations involving the calculation of the Raynal-Revai and the T coefficients [16]. Other approaches for the HH involve introducing intermediate orthogonal subgroups into the group chain. To achieve the invariance under the

rotation, one must transition into the group chain $O_{3N-3} \supset O_3 \otimes S_N$, particularly $O_{3N-3} \supset O_3 \otimes O_{N-1} \supset O_3 \otimes S_N$. The transition allows us to avoid the calculation of the aforementioned coefficients but requires the calculation of the appropriate representation matrices of the orthogonal group and complex algebraic formulations [16].

Naturally, it would be useful to have a relatively simple model describing the nucleus in the intrinsic coordinates that would be suitable for larger systems. This model should use the advantages of a HO basis and be easily employed on the modern high-performance computational resources.

The HO functions are very convenient for the calculations as they can be chosen in such a manner that the transposition of one particle variables induces the orthogonal transformation from one set of the Jacobi coordinates to another. This results in a corresponding expansion with a finite number of terms. If one works with the Jacobi coordinates in the HO basis, then the essential feature is the Talmi-Moshinsky transformation [17, 18] and the corresponding HO brackets [19]. As the number of fermions increases, a larger number of Jacobi coordinates must be transformed and this requires the construction of the higher-order HO transformation brackets [20, 21]. The systematic approach to this problem would be beneficial as it would allow the orderly construction of the translationally invariant state vectors for different nuclei or different clusterization of the nuclei.

There are plenty of approaches for the partition of the nuclei for the state vector construction and one of them is the binary cluster model [22]. The system of N identical particles is divided into two clusters with N_1 and $N_2 = N - N_1$ particles, respectively. When each subcluster has been antisymmetrized, then the two body permutation operator of the symmetric group S_N can be used for the antisymmetrization of the whole system [23]. One can choose the operator P_{1N_1+1}, which interchanges the $1-$st and the N_1+1-th particles. It also transforms Jacobi coordinates and the number of transformed Jacobi coordinates depends on clusterization and the initial antisymmetrization of the N particle system.

Main goal and tasks for the research work

The main goal of this research work is to investigate the description of nuclear systems consisting of six nucleons using the algebraic approach in the translationally invariant basis. The following tasks were formulated:

- Develop an algebraic model for the six nucleon systems in the translationally invariant basis where the system is partitioned as two three-particle subclusters.
  - Formulate a systematic treatment of the transpositions of the Jacobi coordinates and their representations in the HO basis.
  - Create a computationally efficient approach for the accurate state vector construction for the system of six nucleons.
  - Develop generic computational tools for the construction of the antisymmetric state vectors in the translationally invariant HO basis.

Novelty and relevance of the results

In recent years the no core ab-initio methods are being successfully employed to study medium mass nuclei [24]. To model such systems numerically is achievable as the computational power of supercomputers grows due to the rapid technological advances. However, the theoretical developments for the description of such systems are lagging. The advancement in frameworks of the nuclear structure calculations would allow us to explore bigger systems or to do it with less computational resources. The Jacobi coordinate approach in the HO basis for the s-shell nuclei is a popular approach [26] as it allows the explicit center of mass separation. However, for the p-shell nuclei, the M-scheme approach is being usually used due to its simplicity. The six body problem is complex enough for the three-body forces to become significant in the calculation of properties of the nuclei such as Lithium-6. Moreover, this type of system is big enough to check the formulation for the more general case of the binary cluster formalism for the heavier nuclei.

For the six body system, no simplifications appear in the equations as in the description of the simpler systems (for example, four-particle system). In [26] the so-called canonic construction of the fractional parentage coefficients using the antisymmetrization operator is being explored with great success. In this thesis, a different approach is being taken. We employ the symmetric group algebra for the construction of the antisymmetric state vectors in conjunction with the binary cluster formalism, particularly the so-called Λ operators. The Λ operators are constructed from the two-particle transposition operators of the symmetric group. It is a very elegant approach from a theoretical point of view and allows a systematic approach to the nuclear problem. The simplification of the antisymmetrization procedure is achieved by utilizing the symmetry properties of the nuclear system and the isospin formalism. The description of bigger nuclei results in more complex transformations of the Jacobi coordinates and it directly reflects on the representation in the HO basis. This requires computationally efficient generic tools for the calculation of the required transformations.

Statements of the thesis

1. Jacobi coordinates are applicable for the antisymmetric state vector construction for the six nucleon system in the harmonic oscillator basis

2. Coefficients of fractional parentage for the six nucleon systems can be constructed by calculating only one transposition operator of the generating set of the symmetric group S_6.

3. The ab-initio algebraic approach allows constructing the model space for the six nucleon system with reasonable computational resources.

4. The state vector construction in the translationally invariant basis can be done systematically, enabling it to be used efficiently on more complex systems.

Authors contribution and approbation of results

Scientific papers:

1. A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas "HOTB: High precision parallel code for calculation of four-particle harmonic oscillator transformation brackets", Comput. Phys. Commun., Vol. 185, 3062, (2014)

2. D. Germanas, A. Stepšys, S. Mickevičius, R.K. Kalinauskas "HOTB update: Parallel code for calculation of three and four particle harmonic oscillator transformation brackets and their matrices using OpenMP", Comput. Phys. Commun., Vol. 2015, 259, (2017)

3. S. Mickevičius, A. Stepšys , D. Germanas, R.K. Kalinauskas "Calculating fractional parentage coefficients for six body system in translationally invariant basis", Phys. Atom. Nucl., Vol. 81, 899, (2018)

4. A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas "Calculation of orbital fractional parentage coefficients for five particles in translationally invariant basis", Comput. Phys. Commun., Vol. 236, 26, (2019)

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1. LNFK-41 2015, Vilnius: "Šešių kūnų sistemos ab-initio skaičiavimai" (A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

2. Vital Nature Sign 2015, Kaunas: "High precision parallel implementation of four-particle harmonic oscillator transformation brackets for nuclear calculations"; "Ab Initio Calculations Of Six-Body Systems" (A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

3. OpenReadings 2015, Vilnius: "Efficient 9j symbol and harmonic oscillator transformation brackets evaluation for binary cluster calculation" (A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

4. OpenReadings 2016, Vilnius: "Calculation of five particle harmonic-oscillator transformation brackets in translational invariant basis" (A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

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6. OpenReadings 2017, Vilnius: "Construction of antisymmetric basis states for six body systems in translationally invariant basis" (A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

7. LNFK-42 2017, Vilnius: "Kilminių koeficientų skaičiavimas šešių kūnų sistemoms naudojant transliaciškai invariantinę bazę" (A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

8. Advances in Theoretical Nuclear Physics: Probing fundamental interactions by low energy excitations 2017, Stockholm, Sweden: "Antisymmetric basis states construction for six body systems in translationally invariant basis" (A. Stepšys , S. Mickevičius, D. Germanas, R.K. Kalinauskas)

9. OpenReadings 2018, Vilnius: "Different types of clusterization of six body systems using Jacobi coordinates" (A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

10. LNFK-43 2019, Kaunas: "Šešių kūnų sistemos transliaciškai invariantinėje bazėje" (A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

The structure of the thesis

In the first chapter of the thesis, we provide the algebraic approach for the many-body nuclear system. We give the main principles for the construction of the antisymmetric state vectors and the construction of the Hamiltonian for this system. The antisymmetric

state vectors are constructed by using the so-called Λ operator. We debate the importance of the translational invariance and present the technique for the transition from the one particle to the normalized Jacobi coordinates in the isospin formalism. The mathematical tools required to work in the coupled angular momentum basis are described in the section about the angular momentum algebra. In the last section, we introduce the Talmi-Moshinsky transformation.

In the second chapter, the algebraic approach is demonstrated for the construction of the state vectors of the six nucleon system. At first, we construct the coefficients of fractional parentage for the subclusters of this system. Then these coefficients are constructed for the whole system. This procedure is done using the formalism of the Λ operator, presented in the first chapter.

In the third chapter, the higher-order Talmi-Moshinsky transformations are presented. These generic transformations are very useful when two-body permutation elements are calculated and the transformations involving four or five particles are considered. The computational treatment of said coefficients is also discussed in this chapter.

Chapter 1

Description of the nuclear system

1.1 Jacobi coordinates as the intrinsic coordinates of the nucleus

The structure of the nucleus does not depend on the external fields so as a consequence it is required to be translationally invariant. The coordinate responsible for the center of mass (CM) motion must be removed as the nucleus, generally speaking, is an isolated system and does not depend on external fields. For the construction of the correct state vectors, an additional procedure for the elimination of the CM motion needs to be applied. This problem sparks a lot of interest and various methods were developed to solve it [27, 28, 29]. In the NCSM community, this is typically done with the addition of the Lawson term [30] to the Hamiltonian or by the transition to the intrinsic coordinates after the antisymmetrization [31]. For the nuclear systems with $N \leq 4$ constituents the Jacobi coordinates are often used straight away as for the few body systems their application is simple enough. For the $N > 4$ bodies the systems model space is constructed using the three or four body Jacobi coordinate formalism with subclusters antisymmetrized using the Slater Determinants (SDs) [31, 12].

Since the nucleus does not have the definite center of force origin, unlike the atom, the more natural way to describe the nucleus is to use the intrinsic coordinates. These coordinates can be con-

structed as the vectors between the nucleons or the groups of the nucleons [32]. The so-called normalized Jacobi coordinates are expressed though the one particle coordinates $r_1, r_2, ..., r_N$. The transformation from one particle coordinates to the Jacobi coordinates allows the explicit separation of the CM coordinate ρ_0. Moreover, ρ_0 remains invariant under any permutation of $r_1, r_2, ..., r_N$ which induces the orthogonal transformations of the Jacobi coordinates. Basically, there are two approaches to this problem. One can work with one particle variables $(r_1, r_2, ..., r)$ to make the state vectors of the nuclei antisymmetric (for example, by using the SDs). Then the next step is to remove the spurious states, that correspond to the so-called CM excitations.

The other approach is to transform from one-particle variables to the relative coordinate system. The transformation from the one-particle variables to the Jacobi coordinates allows the explicit separation of the CM motion. Non-removal of CM motion gives rise to the nonphysical spurious states [32]. Moreover, the so-called good quantum numbers $J^\pi T$ (total angular momentum, parity, and total isospin) are conserved. The transpositions of the one-particle variables induce orthogonal transformations of the Jacobi coordinates and in general, these transformations must be expressed by an infinite number of terms. The two bases used where these transformations can be represented with a finite number of terms are the HO basis and the Hyperspherical Harmonics (also known as the K-Harmonics, here denoted as HH). The HO basis is widely used in nuclear physics and its popularity can be explained by tradition, its relative simplicity, and years of developed tools. It just works. However, the asymptotics of the HO function is not exactly correct for the wavefunction representation. At a large distance r the HO wavefunction possesses the Gaussian falloff ($\propto e^{-\alpha r^2}$). The actual asymptotics for the wavefunction of the particles bound by the finite-range force is exponential ($\propto e^{-\alpha r}$). As a consequence, the significant excitations of the HO are required for the result to converge [33]. For the one particle variables, the other basis functions are explored [33, 34, 35], however for models where the Jacobi coordinates are being employed the HO or the HH basis are chosen. One particular advantage of the HO basis is the conservation of good quantum numbers in the so-called coupled-J scheme HO

basis. This scheme stands for the basis, where J is a good quantum number as opposed to the M-scheme, where the good quantum number is M, the projection J_z. The coupled J-scheme provides the coupling of the angular momenta of the basis. A consequence of this is a significant reduction of matrix dimensions [14]. Working in a coupled angular momenta basis requires the extensive use of the angular momenta algebra.

The normalized Jacobi coordinates of a given system are constructed according to the Jacobi tree [36]. The Jacobi tree (see fig.(1.1)) is a graph made from $2N-1$ vertices. The $\mathbf{r}_j$ are the one particle coordinates. ρ_0 is the center of mass coordinate and ρ^{12} is the coordinate of the relative motion between the clusters.

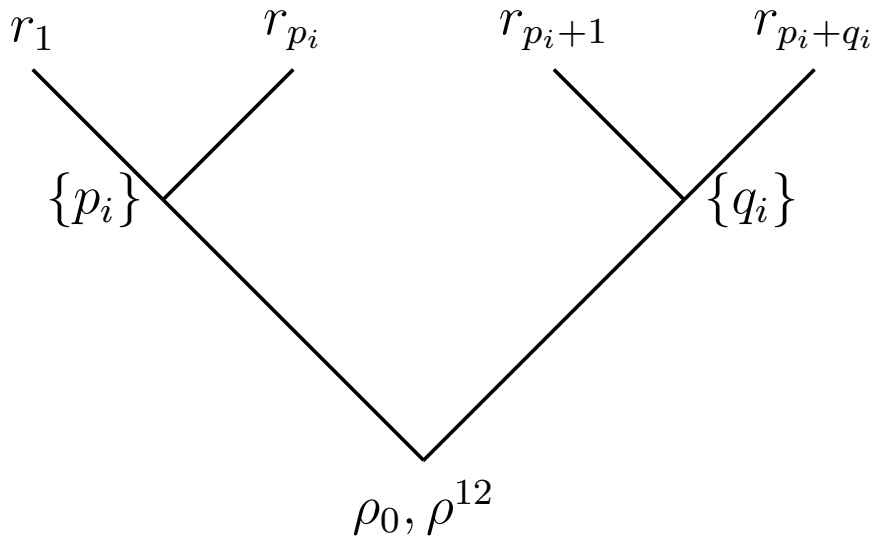


Figure 1.1: The example of the general Jacobi tree

The general expression for the Jacobi coordinate is

$$\rho_i = \sqrt{\frac{p_i q_i}{p_i + q_i}} \left[\frac{1}{p_i} \sum_{j \in \{p_i\}} \mathbf{r}_j - \frac{1}{q_i} \sum_{j \in \{q_i\}} \mathbf{r}_j \right]. \tag{1.1}$$

The first order vertices to the left, are denoted as p_i and the q_i are all the vertices to the right. The Jacobi coordinate system is con-

venient, as the CM motion can be isolated from other coordinates (coordinate ρ_0) :

$$\rho_0 = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \mathbf{r}_j. \tag{1.2}$$

The conversion from $\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N$ to $\rho_0, \rho_1, ..., \rho_{N-1}$ is given by the orthogonal transformation which can be written as matrix. The transformations of the Jacobi coordinates are also orthogonal.

We now have introduced the notation for the Jacobi coordinates, which will be used in the following chapters. If the binary cluster approach is used, then the superscript of the Jacobi coordinate ρ indicates the cluster. The subscript indicates the index of the coordinate of a given subcluster. For example, the second Jacobi coordinate of the first subcluster is denoted as ρ_2^1.

1.2 The formalism of reduced Hamiltonian

For the calculation of the physical properties of the nuclei, one has to construct the Hamiltonian of some sort. The nuclear system consists of the nucleons, who interact upon each other with the strong and electromagnetic forces. The kinetic terms of the Hamiltonian are straightforward, while the potential for the nuclear system is still somewhat a mystery. There is a general consensus that the main terms of the potential energy consist of the two-body interactions. The recent developments in the nuclear theory show that the three-body forces should not be neglected [37].

If one works in the two-particle interaction framework, then the Hamiltonian of the N nucleon system can be written as the sum of all two-body Hamiltonians. In this thesis, the formalism of the reduced Hamiltonian presented in [40] will be used for the six body system ground state energy calculation.

The N body system Hamiltonian with two-body interactions can be written as the sum of the two-body Hamiltonians

$$H = \sum_{i=1<k}^{N} h\left(i,k\right). \tag{1.3}$$

The expression for $h\left(i,k\right)$ can be written as

$$h\left(i,k\right)=-\frac{\hbar^2}{2mN}\left(\nabla_i-\nabla_k\right)^2+V\left(r_i-r_k,\sigma_i\tau_i\sigma_k'\tau_k'\right). \tag{1.4}$$

Eq.(1.4) is known as the reduced Hamiltonian (RH). Here $\hbar$ is the reduced Planck constant, m- the mass of the nucleon, N- the number of the nucleons. The kinetic term depends on the ∇ operator, and generally does not create any problems. On the other hand, the two-body potential term, which depends on the relative distance between the nucleons (r_i-r_k), spin σ, and the isospin τ coordinates of the nucleons is problematic. In general, the potentials of the nuclei are of a phenomenological nature, although in recent years the so-called effective chiral potentials are becoming very popular in the nuclear structure calculations [38, 39]. These potentials are of a theoretical nature and are based on the chiral symmetry breaking.

In the isospin formalism, the protons and the neutrons of the nuclei can be treated as the two states of the same particle. In certain problems, this is reasonable as the isospin symmetry is broken only slightly (a few keV deviation, while the ground state energy of the nuclear system is measured in the MeV range). The mass difference of the proton and the neutron is $|938.28-939.57|=1.39$ Mev/c^2. This difference results only in about 0.147% of the neutron and 0.148% of the proton mass and can be considered negligible. Therefore for the mass of the nucleon one can use the average of the proton and the neutron mass [45] $m=\frac{1}{2}\left(m_n+m_p\right)$. The ratio

$\hbar^2/m$ introduced in the eq.(1.4) is treated as the constant equal to:

$$\frac{\hbar^2}{m}=\hbar\omega\times b^2, \tag{1.5}$$

where $\hbar\omega$ is the harmonic oscillator energy and b is the oscillator length. The observable dependence on $\hbar\omega$ is used more often than dependence on b although these two constants are interchangeable. The dimensionless Jacobi coordinate is introduced as the

$$\rho=\frac{1}{\sqrt{2}b}\left(\mathbf{r}-\mathbf{r}'\right). \tag{1.6}$$

This coordinate connects two particles and its position depends on the chosen Jacobi tree. It also has an explicit dependence on the oscillator length b. The RH can be rewritten using this coordinate as

$$h = -\frac{1}{N}\Delta_\rho + \frac{1}{\hbar\omega} v\left(\sqrt{2}b\rho, \sigma\tau\sigma'\tau'\right), \tag{1.7}$$

where Δ is the Laplace operator acting upon the introduced dimensionless Jacobi coordinate. Eq.(1.7) is called the dimensionless RH. The next procedure is the ρ^2 addition and the subtraction from the dimensionless RH. After term regrouping the dimensionless RH takes shape

$$h = \frac{2}{N}\left[\frac{1}{2}\left(-\Delta_\rho + \rho^2\right)\right] + \left(\frac{1}{\hbar\omega} v\left(\sqrt{2}b\rho, \sigma\tau\sigma'\tau'\right) - \frac{1}{N}\rho^2\right). \tag{1.8}$$

The first group of terms $\left[\frac{1}{2}\left(-\Delta_\xi + \rho^2\right)\right]$ is the Hamiltonian of the harmonic oscillator

$$h_0 = \frac{1}{2}\left(-\Delta_\rho + \rho^2\right). \tag{1.9}$$

The eigenvalues of this Hamiltonian are known. The remaining part can be treated as the difference between the realistic and harmonic oscillator interaction

$$\omega = \frac{1}{\hbar\omega} v\left(\sqrt{2}b\rho, \sigma\tau\sigma'\tau'\right) - \frac{1}{N}\rho^2. \tag{1.10}$$

This simple expression for the RH can be used for any nuclear system when the Schrödinger equation is solved in the HO basis. For the six nucleon system, the RH becomes

$$H_6 = 15\hbar\omega\left(\frac{2}{6}[h_0] + \frac{V\left(\sqrt{2}b\xi_2, \sigma_2\tau_2\sigma_3\tau_3\right)}{\hbar\omega} - \frac{1}{6}\rho^2\right). \tag{1.11}$$

While one can use the isospin formalism to treat the protons and the neutrons of the nuclear system as the same particle, they are most definitely not. You must take into account the correct composition of the nucleus. In the RH formalism, it is done by

tuning the interaction term of the RH expression in such a way that it resembles the certain investigated nuclei. For example, Lithium-6 consists of three protons and three neutrons, while the Berylium-6 contains four protons and two neutrons. One has to take into account the charge dependence of the strong interaction and the Coulomb interaction. The mean nucleon mass of the nucleus can be tuned also according to the structure of the nuclei using the formula $m = \frac{1}{A}(Nm_n + Zm_p)$. For the nucleons, the interaction can have two different isospin states $t = 0, 1$ [45]. When $t = 0$, the projection of the isospin m_t can have only the value zero. This state is called the singlet state. If $t = 1$, then we have the triplet state, with the projection of the isospin m_t acquiring values $-1, 0, 1$. The nucleon-nucleon interaction (or the NN interaction) is different in each state and corresponds to the $V_{PN}(m_t = 0), V_{NN}(m_t = 1), V_{PP}(m_t = -1)$ terms. These three terms correspond to the proton-proton, proton-neutron, and neutron-neutron interactions. Therefore, the two nucleon state can be described as the sum of these potential terms with appropriate coefficients

$$V^{j\pi t}\left(r_{ik}\right) = \sum_{m_t} c_{tm_t} V^{j\pi t m_t}\left(r_{ik}\right), \tag{1.12}$$

where the c_{tm_t} are normalized coefficients

$$\sum_{m_t} c_{tm_t} = 1. \tag{1.13}$$

The values of these coefficients are calculated using the expressions [45]

$$c_{00} = 1, \tag{1.14}$$

$$c_{1-1} = \frac{4Z\left(Z-1\right)}{3A\left(A-2\right)+4T\left(T+1\right)}, \tag{1.15}$$

$$c_{10} = \frac{8NZ - A\left(A+2\right)+4T\left(T+1\right)}{3A\left(A-2\right)+4T\left(T+1\right)}, \tag{1.16}$$

$$c_{1+1} = \frac{4N\left(N-1\right)}{3A\left(A-2\right)+4T\left(T+1\right)}. \tag{1.17}$$

The coefficients for the stable nuclei consisting of six nucleons are presented in the tbl.(1.2).

Table 1.1: The coefficients for the interaction terms for six body systems. Ground state is identified with the quantum numbers $J^\pi T$.

	J	T	c_{1-1}	c_{10}	c_{1+1}
${}^6_1\mathrm{H}_5$	2^-	2	0	$\frac{1}{12}$	$\frac{1}{2}$
${}^6_2\mathrm{He}_4$	0^+	1	$\frac{1}{10}$	$\frac{1}{3}$	$\frac{3}{5}$
${}^6_3\mathrm{Li}_3$	1^+	0	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$
${}^6_4\mathrm{Be}_2$	0^+	1	$\frac{3}{5}$	$\frac{1}{3}$	$\frac{1}{10}$

In this section, the formalism of the RH was introduced, as well as its application to the six nucleon systems. The ground state energy is calculated by computing the Hamiltonian matrix, transforming it into the antisymmetric subspace using the CFPs, and then diagonalizing the resulting matrix. The lowest energy value will correspond to the ground state energy of the system.

1.3 Construction of the antisymmetric subspace

For the description of the nuclear N-body system, the state vectors must satisfy the Pauli principle as the nucleon is a fermion. To ensure the Pauli principle one has to antisymmetrize the wavefunctions or the state vectors. The most popular approach is to use SDs. The SD calculation allows the straightforward construction of the antisymmetric N-body system state vectors depending on the one-particle coordinates $r_1, r_2, ..., r_N$. This gives $3N$ variables to work with while constructing the Hamiltonian. However, for the description of a nucleus, it is sufficient to use $3(N-1)$ variables [32].

1.3.1 Slater determinant and the antisymmetrizer

The multi-fermionic wavefunction must be antisymmetric. This wavefunction can be constructed from one-particle wavefunctions using the Slater determinant. Usually in quantum mechanics textbooks the reader can run into something like this:

$$\Phi_A(x_1, x_2, ..., x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(x_1) & \phi_2(x_1) & ... & \phi_N(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & ... & \phi_N(x_2) \\ ... & ... & ... & ... \\ \phi_1(x_N) & \phi_2(x_N) & ... & \phi_N(x_N) \end{vmatrix} \tag{1.18}$$

This is a general expression for the SD. For simplicity, we now consider the two-particle case

$$\begin{aligned} \Phi_A(x_1, x_2) &= \frac{1}{\sqrt{2!}} \begin{vmatrix} \phi_1(x_1) & \phi_2(x_1) \\ \phi_1(x_2) & \phi_2(x_2) \end{vmatrix} \\ &= \frac{1}{\sqrt{2}}(\phi_1(x_1)\phi_2(x_1) - \phi_1(x_2)\phi_2(x_1)). \end{aligned} \tag{1.19}$$

The resulting expression is an antisymmetric state with the property

$$\Phi_A(x_1, x_2) = -\Phi_A(x_2, x_1). \tag{1.20}$$

An important question is what is the underlying mechanism which makes the determinant formalism work. Let us introduce the antisymmetrizing operator called the antisymmetrizer

$$A_{1,...,N} = \frac{1}{N!} \sum_{P \in S_N} \pi_P P. \tag{1.21}$$

The antisymmetrizer is a sum of the permutation operators of the appropriate symmetric group. The permutation operators transpose the coordinates of the particles. For example, operator P_{12} transposes the coordinates of the first and second particles. δ_P is equal to +1 for an even permutation and -1 for an odd permutation. For the symmetrization of given wavefunctions (if you are working with bosons) there is another operator, called symmetrizer:

$$S_{1,...,N} = \frac{1}{N!} \sum_{P \in S_N} P. \tag{1.22}$$

Antisymmetrizer is a projection operator and has the characteristic that if applied to itself, the operation results in the same operator

$$A * A = A. \tag{1.23}$$

The diagonalization of the projection operator results in eigenvalues of 1 and 0, where the eigenvectors corresponding to the eigenvalue 1 correspond to the transformation into the antisymmetrized state of the system. The antisymmetrizer can be understood as an operator that projects to the antisymmetric subspace.

Let us construct the antisymmetric subspace of a two-particle system. For two particles the antisymmetrizer will use the permutation operators of the symmetric group S_2. This symmetric group contains two operators: the identity operator I and one transposition P_{12}. The antisymmetrizer is equal to

$$A_2 = \frac{1}{2}(1 - P_{12}). \tag{1.24}$$

The application of this operator to the two one particle wavefunctions results in

$$\begin{aligned} A_2\phi_1(x_1)\phi_2(x_2) &= \frac{1}{2}(1 - P_{12})\phi_1(x_1)\phi_2(x_2) \\ &= \frac{1}{2}(\phi_1(x_1)\phi_2(x_2) - P_{12}\phi_1(x_1)\phi_2(x_2)). \end{aligned} \tag{1.25}$$

The operator P_{12} transposes the coordinates of the given wavefunctions

$$A_2\phi_1(x_1)\phi_2(x_2) = \frac{1}{2}(\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1)) \tag{1.26}$$

and the result is the same as using the SD. This toy problem gives us insight into the underlying mechanism of antisymmetrization. The SD is just an easy way to avoid the usage of group theory for antisymmetric subspace construction. However, when you realize that the origin of the SD and antisymmetrization can be explained using group theory, you can use that for a more efficient approach to the antisymmetrization problem, for example, use properties of symmetric groups which is done later in this thesis.

1.3.2 Coefficients of fractional parentage

The coefficients of fractional parentage (CFP) is another traditional technique. In the CFP formalism, the antisymmetric model space is

created from the antisymmetric subsets of the given system. For example, at first, we antisymmetrize a two-particle system and then the deal with a three-particle system. In this case, the antisymmetrized state vectors for the two-particle system can be considered as "parents" for the three-particle states. This approach has the advantage that allows us to deal with smaller systems at first and then gradually move to bigger systems. Moreover, we can significantly reduce the vector space since we do not deal with the whole system at first. The result is smaller matrices, and consequently, we need less computational resources.

The construction of the CFPs for the N nucleon system can be done canonically. In this approach at first the correct state vectors for $N = 2$ are created. Then the state vectors are constructed for the system $N = 3$ and so on until the state vectors for the total system are constructed.

The other way is to work in the binary cluster formalism. This means that the N-body system is divided into the two subclusters of N_1 and $N_2 = N - N_1$ particles with their intrinsic clusterization. Firstly, the CFPs are constructed for the subclusters, then the CFPs for the whole system are constructed [23].

One can approach the CFP construction process by using projection operators, like the antisymmetrizer, discussed in the previous subsection [23]. The antisymmetrizer can be expressed using the much simpler operator X which antisymmetrizes state vectors from the different subclusters

$$A_{1,\ldots,N} = X_{1,..,N_1;N_1+1,\ldots,N} A_{1,\ldots,N_1} A_{N_1+1,\ldots,N}. \tag{1.27}$$

Here the antisymmetrizers of subclusters must be calculated, then the whole system is antisymmetrized. The expression for the operator X can be written as sums of two particle transposition operators

$$X = \begin{pmatrix} N - N_1 \\ N \end{pmatrix} \left\{ 1 + \sum_{j=1}^{\min(N_1, N-N_1)} (-1)^j \times \sum_{l=u_1<u_2<\ldots<u_j}^{N_1} \sum_{N_1+1=v_1<v_2<\ldots<v_j}^{N} P_{u_1 v_1} P_{u_2 v_2} \ldots P_{u_j v_j} \right\} \text{ [25]}. \tag{1.28}$$

The benefit of such an approach is that one does not need to diagonalize the product of these operators in order to get the CFPs. The downside is that one has to work with the full matrices which consist of both physical and non-physical states and this is computationally expensive. Also you have to calculate the sums of the two particle permutation operators and it can be difficult when exploring systems that are heavier than few-body systems.

Another way for the construction of the CFPs is to employ the algebra of the appropriate symmetric group. As the protons and the neutrons of the nucleus are very similar particles, they can be treated as the different states of the same particle, the nucleon. Then the Hamiltonian of a such system is invariant under the permutations of coordinates of the nucleons. As a consequence, the symmetric group S_N can be used to describe the N-nucleon system. Since the isospin symmetry breaking is small compared to the ground state energy of the nucleus, a great simplification can be achieved. For the canonical CFP construction, the group chain

$$S_N \supset S_{N-1} \supset S_{N-2} \supset ... \supset S_1 \tag{1.29}$$

can be used. For the binary cluster system, the group chain is

$$S_N \supset S_{N_1} \times S_{N_2}. \tag{1.30}$$

The appropriate subchains for the $S_{N_1}$and the S_{N_2}depending on the chosen Jacobi coordinate graph must be present.

In this thesis, the operator Λ for the construction of the antisymmetric subspace of the state vectors will be employed. This operator is defined as the sum of all the possible two-body transposition operators P_{ij} of S_N

$$\Lambda = \sum_{i<j=1}^{N} P_{ij}[32]. \tag{1.31}$$

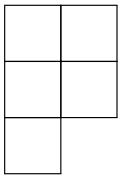
Since all higher-order permutations can be expressed using two-body permutation operators (for example, $P_{123} = P_{12}P_{23}$), the two-body permutations can be understood as the generators of the S_N. All two-body permutation operators of S_N correspond to the character of conjugacy class $\left(1^{N-2}2\right)$.

1.3.3 More terminology from group theory

Two important terms were introduced in the previous subsection: character and conjugacy class. Conjugancy class is a characteristic of a group to distinguish group elements that are connected with the following property. If element a is connected with elements b and c with relation $c = b^{-1}ab$ then the elements are conjugated and correspond to the same class. This important feature as the number of classes in the group corresponds to the irreducible representations of the group. Irreducible representation (or irrep) is a representation that cannot be decomposed. An action of the group can be represented using irreps. Irreps are a way to represent a reducible representation by preserving the information. For example, a full matrix, taking way much space, can be transformed into a block-diagonal form, making the diagonalization of a given matrix way easier. Already discussed group S_2 has two conjugacy classes (1)- no change (the identity element I) and (2)− transposition of two elements (P_{12}). Correspondingly there are two irreducible representations of this group- the symmetric one and the antisymmetric one. Now for a slightly bigger group S_3 one has three conjugacy classes: no change, permutation of two, and the permutation of three elements. Correspondingly, one has three irreps: symmetric, antisymmetric, and mixed symmetry. A common way for the graphical representation of the S_N irreducible representations (irreps) is the Young Diagram (YD) [41]. The standard labeling of the YD $[\lambda] = [\lambda_1, \lambda_2, ..., \lambda_N]$ is in the terms of the Standard Young Tableaux (SYT). The SYT consists of entries $i = 1, ..., N$ filling the Young Diagram corresponding to the representation in all possible ways satisfying the Young rules. An example is presented in fig.(1.2) [42].The character of a class is an invariant number for the particular class. It is equal to the trace of the representation of the group element. To learn more about group theory the reader is referred to the standard texts [42],[43].

1.3.4 Λ operator and its eigenvalues

For the construction of CFPs, we introduced the operator Λ in eq.(1.31). In this subsection, we further explore this operator and show a way to identify the irreps of the symmetric group S_N by



$$[\lambda] = [221].$$

Figure 1.2: A Generic Young Diagram with partition [221]

diagonalizing the matrix of the operator. The eigenvectors are the CFPs. To get the needed eigenvectors, one has to distinguish the irreps, so we need to know which irrep corresponds to which eigenvalue. To determine that we follow the recipe presented in [32]. The character of the class (α) is connected to the sum of all matrix elements of the irreducible representation λ with a relationship

$$\sum_{p\epsilon(\alpha)} D^{\lambda}_{\mu\mu'}(p) = \frac{n(\alpha)}{d_\lambda}\chi^{\lambda}_{(\alpha)}\delta(\mu\mu'). \tag{1.32}$$

Here $n(\alpha)$ is the number of elements of the conjugacy class and d_λ is the dimension of the irrep. λ is the irreducible representation of the S_N. For the class $\left(1^{N-2}2\right)$ for this sum a special notation is introduced connecting the operator Λ and the sum $\Lambda(\lambda)$.

$$\Lambda(\lambda) = \frac{n(n-1)}{2d_\lambda}\chi^{\lambda}_{(1^{N-2}2)} \tag{1.33}$$

The character of the class $\left(1^{N-2}2\right)$ can be calculated using the expression

$$\chi^{\lambda}_{(1^{N-2}2)} = \frac{1}{n(n-1)} d_\lambda \sum_{i=1}^{n} \lambda_i \left(\lambda_i - 2i + 1\right). \tag{1.34}$$

The dimension d_λ can be calculated using the expression

$$d_\lambda = \frac{n! \prod_{i<j=1}^{t} \left(\lambda_i - \lambda_j - i - j\right)}{(\lambda_1 + t - 1)!(\lambda_2 + t - 2)!...\lambda_1!}. \tag{1.35}$$

Here t is the row number. From eq.(1.34) and eq.(1.33) we get the expression

$$\Lambda(\lambda) = \frac{1}{2}\sum_{i=1}^{n}\lambda_i(\lambda_i - 2i + 1). \tag{1.36}$$

Eq.(1.36) allows calculating the eigenvalues of the operator defined in eq.(1.31) for the basis functions represented by the irreducible representation λ of the symmetric group S_N. In eq.(1.36) n is the number of rows in the Young Tableaux and λ_i is the number of boxes of the Young Tableaux in each row.

1.3.5 Coefficients of fractional parentage for binary clusters

In this subsection, we present the CFPs calculation technique for binary clusters using Λ operator. Let us partition N nucleon system into the two subcluster systems consisting of N_1 nucleons and $N_2 = N - N_1$ nucleons. The appropriate symmetric group is S_N and consequently, we have $N - N_1 + 1$ irreps. Only one of them corresponds to a totally antisymmetrical state $[\lambda_1] = \left[1^N\right]$ of the system. The other N_2 representations describe the lower antisymmetric and symmetric representations. We can denote these lower antisymmetry states as $\lambda_{k+1} = \left[2^k 1^{N-2k}\right]$, where $k = 1, ..., N_2$ [44].

The operator Λ is partitioned according to the subclusters. A simple example would be a three-particle system ($N = 3$) factorized into two subclusters $N_1 = 1$ and $N_2 = 2$. Then the symmetric group chain would be

$$S_3 \supset S_1 \times S_2. \tag{1.37}$$

Since the S_1 is trivial let us rewrite the eq.(1.37) as

$$S_3 \supset S_2. \tag{1.38}$$

Subsequently, the expression for Λ would be

$$\Lambda = P_{12} + P_{13} + P_{23} \tag{1.39}$$

The transposition operators P_{23} interchanges the nucleons inside the two- particle subcluster. The operators P_{12} and P_{13} interchange

the nucleons between the subclusters. Let us define the operator Λ correspoding to the subcluster and name the operator as the $\overline{\Lambda}_2(\lambda_2)$. Then we rewrite the expression eq.(1.39) using the operator $\overline{\Lambda}_2(\lambda_2)$

$$\Lambda = P_{12} + P_{13} + \overline{\Lambda}_2(\lambda_2). \tag{1.40}$$

If the subclusters are antisymmetrized, then the operator $\overline{\Lambda}_2(\lambda_2)$ depends only on the irrep $[1^2]$. We can write the expression for Λ as

$$\Lambda = \overline{\Lambda}_2\left(\left[1^2\right]\right) + \sum_{r=1}^{2}\sum_{q=2}^{3} P_{rq}. \tag{1.41}$$

Since we work in the isospin formalism and we have the subclusters antisymmetrized, the transpositions P_{12} and P_{13} will yield the same action, and consequentially we can rewrite the expression from eq.(1.41) as

$$\Lambda = \overline{\Lambda}_2\left(\left[1^2\right]\right) + 2P_{12}. \tag{1.42}$$

Operator responsible for the transposition between the elements of different subclusters can be chosen freely from the aforementioned two transposition elements. This simplification is allowed, because we are working in the antisymmetrized subspaces and therefore the transposition of the nucleon coordinates of the different subclusters transforms as a scalar of the symmetric group S_N.

Let us write the general expression of the operator Λ in the way that it corresponds to the binary division of the N nucleon system $(N = N_1 + N_2)$ [44]:

$$\Lambda = \sum_{i<j=1}^{N_1} P_{ij} + \sum_{l<p=N-N_1+1}^{N} P_{lp} + \sum_{r=1}^{N_1}\sum_{q=N-N_1+1}^{N} P_{rq} \tag{1.43}$$

$$= \overline{\Lambda}_1\left(\left[1^{N_1}\right]\right) + \overline{\Lambda}_2\left(\left[1^{N_2}\right]\right) + N_1N_2P_{1N_1+1}. \tag{1.44}$$

As it was explained in the previous example for three-particle system, the Λ operator can be writen as

$$\Lambda = \overline{\Lambda}_1 (\lambda_1) + \overline{\Lambda}_2 (\lambda_2) + \sum_{r=1}^{N_1} \sum_{q=4-2+1}^{N} P_{rq}. \tag{1.45}$$

Consequently, for the subspaces of the antisymmetric irreps we get the expression

$$\Lambda = \overline{\Lambda}_1 \left(\left[1^{N_1} \right] \right) + \overline{\Lambda}_2 \left(\left[1^{N_2} \right] \right) + N_1 N_2 P_{rq}. \tag{1.46}$$

As in the above example of the three-particles the operator P_{rq} can be chosen freely from the set of intercluster transpositions. The operator P_{1N_1+1} is chosen in this thesis. By using simple algebra the operator P_{1N_1+1} is expressed using Λ operators [44]:

$$P_{1N_1+1} = \frac{1}{N_1 N_2} \left(\Lambda (\lambda) - \overline{\Lambda}_1 \left(\left[1^{N_1} \right] \right) - \overline{\Lambda}_2 \left(\left[1^{N_2} \right] \right) \right). \tag{1.47}$$

By having antisymmetric subspaces, the number of the spawned irreps from those subspaces can be only of two types: $\lambda_{k+1} = [2^k 1^{N-2k}]$, $\left[1^N \right]$. The algebraic expressions for the eigenvalues of the diagonalized operator P_{1N_1+1} corresponding these to these irreps are

$$P_{1N_1+1}|_{\lambda=[1^N]} = -1 \tag{1.48}$$

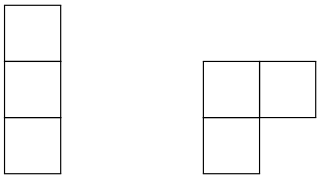
and

$$P_{1N_1+1}|_{\lambda=\left[2^k 1^{N-2k}\right]} = \frac{1}{N_1 N_2} [(k - N_1) N - k (k-1) + N_1^2]. \tag{1.49}$$

The eigenvectors of the operator P_{1N_1+1}, corresponding to the eigenvalue of the irrep $[1^N]$ are the desired CFPs of the N-nucleon system. The Λ operator for the three-particle system was constructed above. If one has the antisymmetrized subcluster that corresponds to the symmetric group S_2 irrep $[1^2]$ then the possible irreps spawned by the Λ operator would be $[1^3]$ and $[21]$. The Young diagram representation of such irreps is presented in fig.(1.3).

1.4 Angular momentum algebra

In this thesis, the state vectors will be constructed in the coupled-J basis. The upside of this basis is that it has significantly lower



$a)[\lambda_1] = [1^3]$ $\quad$ $b)[\lambda_2] = [21]$

Figure 1.3: The Young Diagrams corresponding to the irreps of S_3. a) corresponds to the totally antisymmetric irrep $[1^3]$ and b) corresponds to the irrep with lesser degree of antisymmetry [21].

dimensions that the M-scheme. The downside is that working in this framework requires intensive use of the angular momentum recoupling coefficients (REC). Two uncoupled angular moments j_1 and j_2 with projections m_1 and m_2 can be coupled into the total angular momentum J with projection M. This is done by using the completeness relation

$$\sum_{\alpha} |\alpha\rangle \langle\alpha| = I. \tag{1.50}$$

Here I is the identity operator and $|\alpha\rangle \langle\alpha|$ defines arbitrary orthonormal state vectors. This relation is very simple yet powerful as it allows us to expand some arbitrary basis through some orthonormal expansion coefficients. For example, lets say we have some basis $|\beta\rangle$ and we want to transform it to the basis $|\alpha\rangle$ .This can be done using the relation from eq.(1.50)

$$|\beta\rangle = \sum_{\alpha} |\alpha\rangle \langle\alpha|\beta\rangle \,, \tag{1.51}$$

where $\langle\alpha|\beta\rangle$ is the expansion coefficients. In our angular momentum scenario, these coefficients are called the Clebsch-Gordan coefficients (CG)

$$|JM\rangle = \sum_{\substack{m_1=[-j_1,j_1] \\ m_2=[-j_2,j_2]}} |j_1 m_1 j_2 m_2\rangle \langle j_1 m_1 j_2 m_2|JM\rangle \,. \tag{1.52}$$

They are also often denoted as $C^{JM}_{j_1 m_1, j_2 m_2}$.This notation I will be using in this thesis if not stated otherwise. The CGs are equal to zero if the following conditions are not met. The triangular rule

$$|j_1 - j_2| < J < j_1 + j_2, \tag{1.53}$$

and the condition

$$m_1 + m_2 = M. \tag{1.54}$$

The quantum numbers j_1, j_2, J must be integral or half-integral numbers and the same goes for m_1, m_2, M, which can also be positive and negative. The modules of the projections m_1, m_2, M cannot be greater than j_1, j_2, J and the sums $j_1 + m_1, j_2 + m_2, J + M, j_1 + j_2 + J$ must be integral and non-negative.

Another similar coefficient is the Wigner 3jm symbol. They are connected by a simple relation

$$C^{JM}_{j_1 m_1, j_2 m_2} = (-1)^{j_1 - j_2 + m_3} \sqrt{2J+1} \begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & -M \end{pmatrix}. \tag{1.55}$$

Essentially, the Clebsch-Gordan coefficient can be understood as the 3jm symbol with a phase and dimension multipliers. The abreviation d_{x_y} will be used for the dimensional multiplier of type $(2x_y + 1)$, where y is a number. By itself, this symbol is not orthonormal and can be understood as the probability amplitude that the angular momenta j_1, j_2, J with their projections sum up into zero angular momentum state $|00\rangle$

$$\begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & M \end{pmatrix} = (-1)^{j_1 - j_2 + J} \sum_{j'm'} C^{J'M'}_{j_1 m_1, j_2 m_2} C^{00}_{j'm', JM} \text{ [46]}. \tag{1.56}$$

The 3jm symbols are more convenient as they possess much simpler symmetry relations than the CGs. For example, the 3jm symbol is invariant under the even permutation of its columns and odd permutation would yield only one additional phase multiplier. The CGs do not have this property and the permutation of j_x would result not only in phase multipliers but in additional dimensional multipliers and the change of sign of the projection quantum number. For example,

$$C^{JM}_{j_1 m_1, j_2 m_2} = (-1)^{j_1 - m_1} \sqrt{\frac{d_J}{d_{j_1}}} C^{j_2, -m_2}_{j_1 m_1, J, -M}. \tag{1.57}$$

The symmetry properties of the CGs can make calculations significantly harder than they have to be.

When more angular momenta are coupled, an intermediate angular momentum quantum number must be introduced. Let us say we have angular momenta j_1, j_2, j_3, which are coupled into total angular momentum J. Then one of the possible coupling schemes is $|((j_1, j_2)j_{12}, j_3)JM\rangle$ with intermediate j_{12}. The other possible scheme is $|((j_1, (j_2, j_3)j_{23})JM\rangle$ with j_{23}. RECs who allow transitioning between these two couplings involve a so-called 6j symbol with an appropriate dimensional multiplier

$$\begin{aligned} &\langle((j_1, j_2)j_{12}, j_3)JM|((j_1, (j_2, j_3)j_{23})JM\rangle \\ &= (-1)^{j_1+j_2+j_3+J} \sqrt{d_{j_{12}} d_{j_{23}}} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & J & j_{23} \end{Bmatrix} \delta_{jm,j'm'}. \end{aligned} \tag{1.58}$$

Function $\delta_{jm,j'm'}$ is defined as the two standard Dirac delta functions of the type $\delta_{x,x'}$, where x is a quantum number. For three js there are two more coefficients-

$$\langle((j_1, j_2)j_{12}, j_3)JM|((j_1, j_3)j_{13}, j_2)JM\rangle \tag{1.59}$$

and

$$\langle((j_1, (j_2, j_3)j_{23})JM|((j_1, j_3)j_{13}, j_2)JM\rangle\,, \tag{1.60}$$

who possess the same structure. The 6j symbol can be understood as the sums of a series of CGs by their projections m_x for fixed M and M'

$$\begin{aligned} &\langle((j_1, j_2)j_{12}, j_3)JM|((j_1, (j_2, j_3)j_{23})JM\rangle \\ &= \sum C^{JM}_{j_{12} m_{12}, j_3 m_3} C^{j_{12} m_{12}}_{j_1 m_1, j_2 m_2} C^{j' m'}_{j_1 m_1, j_{23} m_{23}} C^{j_{23} m_{23}}_{j_2 m_2 j_3 m_3} \\ &= (-1)^{j_1+j_2+j_3+J} \sqrt{d_{j_{12}} d_{j_{23}}} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & J & j_{23} \end{Bmatrix} \delta_{jm,j'm'}. \end{aligned} \tag{1.61}$$

There is a similar formula for the summation of the 3jm coefficients, which result in a 6j symbol without the phase and dimension multipliers. The 6j symbols are highly symmetric- invariant under

permutations of columns and if upper and lower arguments are interchanged in any of the two columns. They are equal to zero if the triangular rule is not satisfied for triads (j_1, j_2, j_{12}), (j_{12}, j_3, j_{23}), (j_{12}, j_3, j_{23}), (j_{23}, j_1, J).

For the recoupling of the four angular momenta, the coefficients follow the same construction. For example, the recoupling from the vector state

$$|((j_1, j_2)j_{12}, (j_3, j_4)j_{34})JM\rangle \tag{1.62}$$

to

$$|((j_1, j_3)j_{13}, (j_2, j_4)j_{24})JM\rangle \tag{1.63}$$

results in

$$\begin{aligned}&\langle((j_1, j_2)j_{12}, (j_3, j_4)j_{34})JM|((j_1, j_3)j_{13}, (j_2, j_4)j_{24})JM\rangle \\ &= \sqrt{d_{j_{12}} d_{j_{13}} d_{j_{24}} d_{j_{34}}} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & J \end{Bmatrix} \delta_{jm,j'm'}.\end{aligned} \tag{1.64}$$

The curly bracket is the 9j symbol. Like the 6j symbol, it can be understood as multiple sums of the CGs by the angular momentum projections. This symbol is invariant for even permutation of the columns or rows of the parameters as well as the transposition of the symbol. The odd permutation yields a phase multipler $(-1)^x$, where x is the sum of all the parameters of the symbol. The 9j symbol can be calculated by using the standard expression of the reduction of the 9j symbol to the sum of the three 6j symbols

$$\begin{aligned}\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \\ k_1 & k_2 & k_3 \end{Bmatrix} &= \sum_x (-1)^{2x} (2x+1) \\ \times \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_3 & k_3 & x \end{Bmatrix} &\begin{Bmatrix} l_1 & l_2 & l_3 \\ j_2 & x & k_2 \end{Bmatrix} \begin{Bmatrix} k_1 & k_2 & k_3 \\ x & j_1 & l_1 \end{Bmatrix}.\end{aligned} \tag{1.65}$$

In the phase multiplier $(-1)^{2x}$ the power of 2 is kept since the values of angular momenta can be half-integer. There are also higher-order symbols like 12j, 15j, and so on. Due to their complicated nature, these symbols are rarely used. For more about the angular momentum algebra, the reader is referred to [46].

1.4.1 The square bracket notation

As stated before, while working in a coupled-j basis you need to use a lot of RECs. As a result, the expressions can become quite complicated so it is very practical to have a methodical approach for them. For this purpose, we introduce the square bracket notation. The coefficients for the recoupling of the four angular momenta in the bra-ket notation are denoted as

$$\langle((j_1,j_2)J_{12},(j_3,j_4)J_{34})J|((j_1,j_3)J_{13},(j_2,j_4)J_{24})J\rangle\,. \tag{1.66}$$

For the intermediate and the final angular momentum we will use capital letters. We rewrite them in 3 by 3 matrix with the square brackets following the 9j symbol structure as

$$\langle((j_1,j_2)J_{12},(j_3,j_4)J_{34})J|((j_1,j_3)J_{13},(j_2,j_4)J_{24})J\rangle = \begin{bmatrix} j_1 & j_3 & J_{13} \\ j_2 & j_4 & J_{24} \\ J_{12} & J_{34} & J \end{bmatrix}. \tag{1.67}$$

This recoupling coefficient is calculated using the 9j symbol

$$\begin{bmatrix} j_1 & j_3 & J_{13} \\ j_2 & j_4 & J_{24} \\ J_{12} & J_{34} & J \end{bmatrix} = \sqrt{d_{J_{12}}d_{J_{34}}d_{J_{13}}d_{J_{24}}} \begin{Bmatrix} j_1 & j_3 & J_{13} \\ j_2 & j_4 & J_{24} \\ J_{12} & J_{34} & J \end{Bmatrix}. \tag{1.68}$$

If one of the values in the matrix $\begin{bmatrix} j_1 & j_3 & J_{13} \\ j_2 & j_4 & J_{24} \\ J_{12} & J_{34} & J \end{bmatrix}$ is equal to zero, i.e. $\begin{bmatrix} j_1 & 0 & J_{13} \\ j_2 & j_4 & J_{24} \\ J_{12} & J_{34} & J \end{bmatrix}$, then this coefficient recouples only three angular momentum values. In this case the recoupling coefficient is expressed using the 6j symbol, as the 9j symbol reduces to the 6j symbol if one of its values in 3 by 3 matrix is zero.

This type of notation is very convenient as it allows to keep track of changes of the basis vector. To recouple the basis vector $\langle((j_1,j_2)J_{12},j_3)J|$ to $|((j_1,(j_2,j_3)J_{23})J\rangle$ we use the recoupling coefficient with one zero value :

$$\langle((j_1,j_2)J_{12},j_3)J|((j_1,(j_2,j_3)J_{23})J\rangle = \begin{bmatrix} j_1 & 0 & j_1 \\ j_2 & j_3 & J_{23} \\ J_{12} & j_3 & J \end{bmatrix} \tag{1.69}$$
$$= \sqrt{d_{J_{12}} d_{j_1} d_{J_{23}} d_{j_3}} \begin{Bmatrix} j_1 & 0 & j_1 \\ j_2 & j_3 & J_{23} \\ J_{12} & j_3 & J \end{Bmatrix}.$$

Since the 9j symbol contains zero, the expression in eq.(1.69) can be simplified by the reduction of the 9j symbol to the 6j symbol

$$\sqrt{d_{J_{12}} d_{j_1} d_{J_{23}} d_{j_3}} \begin{Bmatrix} j_1 & 0 & j_1 \\ j_2 & j_3 & J_{23} \\ J_{12} & j_3 & J \end{Bmatrix} \tag{1.70}$$
$$= \sqrt{d_{J_{12}} d_{j_1} d_{J_{23}} d_{j_3}} \frac{(-1)^{j_2+J+j_3+j_1}}{\sqrt{d_{j_3} d_{j_1}}} \begin{Bmatrix} J_{23} & J & j_1 \\ J_{12} & j_2 & j_3 \end{Bmatrix}$$
$$= (-1)^{j_2+J+j_3+j_1} \sqrt{d_{J_{12}} d_{J_{23}}} \begin{Bmatrix} J_{23} & J & j_1 \\ J_{12} & j_2 & j_3 \end{Bmatrix}$$
$$= (-1)^{j_2+J+j_3+j_1} \sqrt{d_{J_{12}} d_{J_{23}}} \begin{Bmatrix} j_1 & j_2 & J_{12} \\ j_3 & J & J_{23} \end{Bmatrix}.$$

The final expression for the recoupling coefficient is

$$\langle((j_1,j_2)J_{12},j_3)J|((j_1,(j_2,j_3)J_{23})J\rangle = \begin{bmatrix} j_1 & 0 & j_1 \\ j_2 & j_3 & J_{23} \\ J_{12} & j_3 & J \end{bmatrix} \tag{1.71}$$
$$= (-1)^{j_2+J+j_3+j_1} \sqrt{d_{J_{12}} d_{J_{23}}} \begin{Bmatrix} j_1 & j_2 & J_{12} \\ j_3 & J & J_{23} \end{Bmatrix}.$$

The same approach is used for the calculation of the reversed recoupling coefficient $\langle((j_1,(j_2,j_3)J_{23})J|((j_1,j_2)J_{12},j_3)J\rangle$. This coefficient results in a matrix with a zero on the left part of the square bracket

$$\begin{bmatrix} j_1 & j_2 & J_{12} \\ 0 & j_3 & j_3 \\ j_1 & J_{23} & J \end{bmatrix}. \tag{1.72}$$

The expression for this coefficient follows the same rules as in the eq.(1.70) and results in expression

$$\begin{bmatrix} j_1 & j_2 & J_{12} \\ 0 & j_3 & j_3 \\ j_1 & J_{23} & J \end{bmatrix} = (-1)^{0+j_3-j_3}\sqrt{d_{j_1}d_{J_{23}}d_{j_3}d_{J_{12}}} \begin{Bmatrix} j_1 & j_2 & J_{12} \\ 0 & j_3 & j_3 \\ j_1 & J_{23} & J \end{Bmatrix} \tag{1.73}$$

$$= \sqrt{d_{j_1}d_{J_{23}}d_{j_3}d_{J_{12}}}\frac{(-1)^{j_2+J+j_3+j_1}}{\sqrt{d_{j_3}d_{j_1}}} \begin{Bmatrix} J_{23} & j_2 & j_3 \\ J_{12} & J & j_1 \end{Bmatrix}$$

$$= (-1)^{j_2+J+j_3+j_1}\sqrt{d_{J_{23}}d_{J_{12}}} \begin{Bmatrix} j_3 & j_2 & J_{23} \\ j_1 & J & J_{12} \end{Bmatrix}.$$

The square matrix notation for the recoupling coefficients will be used in the future formulae if not stated differently. This notation allows to easily keep track of the indices aswell as the structure of the coefficients.

1.5 The Talmi-Moshinsky transformation

In subsection 1.3.4 we discussed the construction of CFPs using the Λ operator. As we want to employ the harmonic oscillator in our nuclear calculations, we need to have tools to construct Λ operator representation in the harmonic oscillator basis. The nucleus has to be described with good quantum numbers. For Jacobi coordinates the convenient set of good quantum numbers is $J^\pi T$. J denotes the total angular momentum of the nucleus, π is parity, and T is the isospin. The total angular momentum of the nuclei contains terms of orbital angular momentum L and spin part (denoted as S). The state vectors of the system must be antisymmetrized to respect all quantum numbers. The antisymmetrization of the state vectors for the spin and the isospin will be discussed later in Chapter 2. In this section, we will concentrate on the orbital part, which is governed by angular momentum.

In the Jacobi coordinate basis the construction of the antisymmetrized state vectors requires dealing with the transpositions of the one-particle variables $(r_1, r_2, ..., r)$. These transpositions induce the orthogonal transformations of the Jacobi coordinates, generally

known as the Talmi-Moshinsky (TM) transformation. In the HO basis, these orthogonal transformations can be represented with a finite number of terms. The tool to represent these transformations in HO basis is the harmonic oscillator transformations brackets (HOB) also known as the Talmi-Moshinsky or the Talmi-Moshinsky-Smirnov brackets (TMB). In this thesis to tackle HOBs we follow [47]. The TM transformation is the orthogonal transformation characterized by the SO_2 group. Standard TM transformation in the coordinate basis is defined as the two–dimensional matrix

$$\begin{pmatrix} \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} \\ \sqrt{\frac{1}{1+d}} & -\sqrt{\frac{d}{1+d}} \end{pmatrix}, \tag{1.74}$$

where the parameter d is a nonnegative real number. This matrix is analogous to the matrix

$$\begin{pmatrix} \sin(\theta) & \cos(\theta) \\ \cos(\theta) & -\sin(\theta) \end{pmatrix}, \tag{1.75}$$

where θ is the Euler angle. The transformation acts on the coordinate vector $\begin{pmatrix} r_1 \\ r_2 \end{pmatrix}$ and results in the transformed vector $\begin{pmatrix} r'_1 \\ r'_2 \end{pmatrix}$. The representation of this transformation in the HO basis, HOBs is denoted as $\langle e_1 l_1, e_2 l_2 : L | e'_1 l'_1, e'_2 l'_2 : L \rangle_d$ [47]. Here $e_1 l_1, e_2 l_2$ are quantum numbers of the energy and the angular momentum of the HO corresponding to the aforementioned coordinates $r_1$and r_2.

The properly orthonormalized HO function for the wavefunction approximation is

$$\phi_{elm}(\mathbf{r}) = (-1)^n \left[\frac{2\,(n!)}{\Gamma\,(n+l+3/2)} \right]^{\frac{1}{2}} e^{\left(-r^2/2\right)} r^l L_n^{(l+1/2)}\left(r^2\right) Y_{lm}(\mathbf{r}/r)\,. \tag{1.76}$$

$L_n^{(l+1/2)}$ is the generalized Laguerre polynomial and $Y_{lm}(\mathbf{r}/r)$ are the spherical harmonics. Γ is the gamma function. The HOBs are a highly symmetric tool with conserved quantum numbers. The energy conservation rule is $e_1+e_2 = e'_1+e'_2$ and the angular momentum quantum numbers must satisfy the relation $(-1)^{l_1+l_2} = (-1)^{l'_1+l'_2}$. The connection between the quantum number e and the quantum number n is $n = \frac{(e-l)}{2}$.

The two-particle wavefunction is constructed by coupling the wavefunctions using Clebsch-Gordan coefficient $\langle l_1 m_1, l_2 m_2 \,|\Lambda\lambda\rangle$

$$\begin{aligned} |e_1 l_1 (\mathbf{r}_1), e_2 l_2 (\mathbf{r}_2) : \Lambda\lambda\rangle &\equiv \{\phi_{e_1 l_1} (\mathbf{r}_1) \otimes \phi_{e_2 l_2} (\mathbf{r}_2)\}_{\Lambda\lambda} \\ &= \sum_{m_1 m_2} \langle l_1 m_1, l_2 m_2 \,|\Lambda\lambda\rangle \, \phi_{e_1 l_1 m_1} (\mathbf{r}_1) \, \phi_{e_2 l_2 m_2} (\mathbf{r}_2) \end{aligned} \tag{1.77}$$

and HOBs are defined as the transformation

$$\begin{aligned} |e_1 l_1 (\mathbf{r}_1), e_2 l_2 (\mathbf{r}_2) : \Lambda\lambda\rangle = \sum_{EL,el} &\langle EL, el : \Lambda \,|e_1 l_1, e_2 l_2 : \Lambda\rangle_d \\ &\times |EL (\mathbf{R}), el (\mathbf{r}) : \Lambda\lambda\rangle . \end{aligned} \tag{1.78}$$

HOBs are equal to zero, unless the angular momenta satisfies the triangle conditions. The triangle conditions come from the angular momenta algebra and are explicitly defined as

$$|l_1 - l_2| \leq L \leq l_1 + l_2 \tag{1.79}$$

$$|l'_1 - l'_2| \leq L \leq l'_1 + l'_2 \tag{1.80}$$

The value of the coupled angular momenta L cannot be greater than the sum of the values of the separate angular momenta quantum numbers l_1 and l_2. Also it cannot be lower than the modulus of a difference between them. HOBs are highly symmetric and the symmetry relations for the them are as follows

$$\langle e_1 l_1, e_2 l_2 : L | e'_1 l'_1, e'_2 l'_2 : L\rangle_d = \tag{1.81}$$

$$\langle e'_1 l'_1, e'_2 l'_2 : L \,|e_1 l_1, e_2 l_2 : L\rangle_d = \tag{1.82}$$

$$(-1)^{l'_1 + l_2} \langle e_2 l_2, e_1 l_1 : L \,|e'_2 l'_2, e'_1 l'_1 : L\rangle_d = \tag{1.83}$$

$$(-1)^{L - l'_1} \langle e_2 l_2, e_1 l_1 : L \,|e'_1 l'_1, e'_2 l'_2 : L\rangle_{1/d} = \tag{1.84}$$

$$(-1)^{L - l_1} \langle e_1 l_1, e_2 l_2 : L \,|e'_2 l'_2, e'_1 l'_1 : L\rangle_{1/d} \ . \tag{1.85}$$

The absolute value of HOB does not change if the parameters are interchanged (eqs.(1.81,1.82,1.83)). Only the sign of the value can be flipped in cases presented in eqs.(1.83,1.84,1.85). Also the value of HOB does not change if d is inverted (eqs.(1.84,1.85)).These symmetry properties allow a significant speedup of the calculations

where the HOBs are employed. HOBs are orthogonal and normalized coefficients:

$$\sum_{EL,el} \langle e_1 l_1, e_2 l_2 : \Lambda \,|EL, el : \Lambda\rangle_d \langle EL, el : \Lambda \,|e_1' l_1', e_2' l_2' : \Lambda\rangle_d = \delta_{e_1 l_1, e_1' l_1'} \delta_{e_2 l_2, e_2' l_2'}. \tag{1.86}$$

The general expressions for calculating HOBs are discussed by a number of authors [48, 49, 50]. B.Buck and A.C. Merchan presented an expression for direct calculation of the TMB in [51]:

$$\begin{aligned}
&\langle EL, el : \Lambda \,|e_1 l_1, e_2 l_2 : \Lambda\rangle_d \qquad (1.87)\\
&= i^{-(l_1+l_2+L+l)} \times 2^{-(l_1+l_2+L+l)/4}\\
&\times \sqrt{(n_1)!\,(n_2)!\,(N)!\,(n)!\,[2(n_1+l_1)+1]!!\,[2(n_2+l_2)+1]!!}\\
&\times \sqrt{[2(N+L)+1]!!\,[2(n+l)+1]!!} \sum_{abcdl_a l_b l_c l_d} (-1)^{l_a+l_b+l_c}\\
&\times 2^{(l_a+l_b+l_c+l_d)/2} d^{(2a+l_a+2d+l_d)/2} (1+d)^{-(2a+l_a+2b+l_b+2c+l_c+2d+l_d)/2}\\
&\times \frac{[(2l_a+1)(2l_b+1)(2l_c+1)(2l_d+1)]}{a!b!c!d!\,[2(a+l_a)+1]!!\,[2(b+l_b)+1]!!\,[2(c+l_c)+1]!!\,[2(d+l_d)+1]!!}\\
&\times \left\{ \begin{array}{ccc} l_a & l_b & l_1 \\ l_c & l_d & l_2 \\ L & l & \Lambda \end{array} \right\} \langle l_a 0 l_c 0|\, L0\rangle \langle l_b 0 l_d 0|\, l0\rangle \langle l_a 0 l_b 0|\, l_1 0\rangle \langle l_c 0 l_d 0|\, l_2 0\rangle ,
\end{aligned}$$

where $N = (E-L)/2$, $n = (e-l)/2$, $n_1 = (e_1 - l_1)/2$, and $n_2 = (e_2 - l_2)/2$. In [47] this expression was rewritten to make it computationally more efficient

$$\begin{aligned}
&\langle EL, el : \Lambda \,|e_1 l_1, e_2 l_2 : \Lambda\rangle_d \qquad (1.88)\\
&= d^{(e_1-e)/2} (1+d)^{-(e_1+e_2)/2} \sum_{e_a l_a e_b l_b e_c l_c e_d l_d} (-d)^{e_d} \left\{ \begin{array}{ccc} l_a & l_b & l_1 \\ l_c & l_d & l_2 \\ L & l & \Lambda \end{array} \right\}\\
&\times G(e_1 l_1; e_a l_a, e_b l_b)\, G(e_2 l_2; e_c l_c, e_d l_d)\, G(EL; e_a l_a, e_c l_c)\, G(el; e_b l_b, e_d l_d) .
\end{aligned}$$

Here the 3 by 3 matrix in the curly brackets is the 9j symbol. The function G is calculated as

$$G\left(e_1 l_1; e_a l_a, e_b l_b\right) = \sqrt{\left(2l_a+1\right)\left(2l_b+1\right)}\left\langle l_a 0 l_b 0 \right| l_1 0\rangle \times \left[\begin{pmatrix} e_1 - l_1 \\ e_a - l_a; e_b - l_b \end{pmatrix}\begin{pmatrix} e_1 + l_1 + 1 \\ e_a + l_a + 1; e_b + l_b + 1 \end{pmatrix}\right]^{1/2} \tag{1.89}$$

where the coefficients

$$\begin{pmatrix} n_1 \\ n_a; n_b \end{pmatrix} = \frac{(n_1)!!}{(n_a)!!\,(n_b)!!} \tag{1.90}$$

are the trinomial coefficients defined for $n_1 \geq n_a, n_b$. The other additional coefficient is the CG with angular momenta projection equal to zero

$$\left\langle l_1 0 l_2 0 \right| l 0\rangle = (-1)^{(l_1+l_2-l)/2}\left[\binom{2l}{l_1 - l_2 + l}\binom{l_1 + l_2 + l + 1}{2l+1}\right]^{-1/2} \times \binom{l}{\left(l_1 - l_2 + l\right)/2}\binom{\left(l_1 + l_2 + l\right)/2}{l}. \tag{1.91}$$

In eq.(1.91) brackets define the binomial coefficients. The 9j symbol is calculated using the eq.(1.65). The presented expressions will be used extensively for the calculations of the HOB coefficients in this thesis. A Fortran code [47] using this approach for HOB calculation is well known and widely used(for example, in [52, 53, 37]).

1.5.1 Evaluation of the 6j symbols

The cornerstone of the calculations in coupled-J basis is the use of angular momenta recoupling coefficients. These coefficients as well as HOBs are expressed using the 6j and 9j symbols. The standard expressions for calculating these so called 3nj symbols (an umbrella term for 3j, 6j, and higher-order symbols) involves complicated sums of factorial terms (see [46] for explicit formulae). The eq.(3.5) for calculation of HOBs has a heavy dependence on 9j symbol. 9j symbol is calculated by summing three 6j symbols

(eq.(1.70)). These symbols are calculated using eq.(1.88) which has a dependence on the binomial coefficients instead of factorials. This makes it more suitable for the calculation on the computer. Especially using the double precision variables. Although numerically more stable that the standard expressions it starts to produce significant errors when the total harmonic oscillator energy becomes equal to 25 [54].

The heavy dependence on the symbols reflects in the computer code. Simple profiling of serial Fortran code for the P_{14} element evaluation shows that the percentage of the running time spent in function for the calculation of the 6j symbols adds up to 55% of the total running time. So the question arises, are there other ways to calculate the required symbols faster and give smaller errors. For this purpose, several computer codes for the calculation of the 6j and 9j symbols were explored [55, 56, 57]. In the approach by L.Wei [56] the 6j and 9j symbols are reformulated in a form of a product of two factors. One is the square root of integer products and quotients and the other is the summation of the products of binomial coefficients. Two types of number representation are used. The prime number representation for the first factor and the 32768-base number representation for the summation terms. The following representation is useful when the summation terms involve huge integer numbers. In the tables (1.2) and (1.3) this algorithm is denoted as Wei. The next approach described in [55] also utilizes the binomial coefficients for the 3j and the 6j symbols. The presented code has two ways for calculation of the symbols: the direct summation of the binomial coefficients and the recursive approach. These two methods are denoted in the tables as TuzunDirect and TuzunRecursive. The last one [57] uses precalculated tables for the lookup of the 6j and 9j symbols. It will be denoted by its name FASTWIGXJ. In this library for the 3j and 6j symbols, the lookup table is organized by the direct indexing using Reggies symmetries[58] and for the 9j symbols, the values are stored in the hash table. The values of symbols are calculated using another code from the same authors called WIGXJPF[59]. We precalculated the 6j symbols up to $j = 30$ and the 9j symbols up to $j = 20$. The file for 6j symbols takes 15 Mb of storage while the 9j symbol file is 1.1 Gb. For this library, we did one benchmark with

the precalculated 9j symbols and the other one with precalculated 6j symbols to be used with formula from eq.(1.65).

We used these algorithms in HOB matrix calculation, to compare speed and bias. Bias is evaluated by exploiting the fact that the HOB matrix is orthonormal, thus possess the property $HOB * HOB^T = I$, where I is the identity matrix. We calculate the deviation from an ideal identity matrix and thus get the bias. We can clearly see in the tbl.(1.2) than the algorithm described in previous section (denoted as "Bin") starts to produce signifficant errors at the HO energy equal to 20. Other algorithms are clearly more stable, producing errors at the same order of magnitude, ergo they are comparable. The most precise is the library WIGXJPF. From tbl.(1.3) we see that while precise the slowest approach was by L.Wei. The second slowest was the FASTWIGXJ with 6j symbol tabulation and the third slowest with 9j symbol tabulation. It appears that even if the symmetries of the symbols are exploited and they are efficiently tabulated, the price for search is too high. Keeping that in mind and that an approach by R. E. Tuzun et al. was fairly fast and produced good results, we can say that computer code is the best choice if one needs fast computation with a minimal tradeof of precision.

Table 1.2: 3HOB calculation bias using different approaches for 9j symbol evaluation. E is the energy of the HO; L is equal to E/2; Dim is the dimension of matrix.

E	Dim	Bin	Wei	$TuzDir$	$TuzRec$	$WigXj6j$	$WigXj9j$
4	9	3.02×10^{-14}	7.19×10^{-15}	1×10^{-14}	1×10^{-14}	1.02×10^{-14}	7.19×10^{-15}
6	9	4.5×10^{-14}	5.55×10^{-15}	8.55×10^{-15}	8.8×10^{-15}	7.12×10^{-15}	6.66×10^{-15}
8	30	6.39×10^{-12}	6.05×10^{-14}	7.36×10^{-14}	7.67×10^{-14}	8.08×10^{-14}	6.05×10^{-14}
10	30	1.8×10^{-11}	6.12×10^{-14}	7.05×10^{-14}	7.43×10^{-14}	7.92×10^{-14}	5.47×10^{-14}
12	70	1.39×10^{-9}	4.34×10^{-13}	5.19×10^{-13}	5.32×10^{-13}	5.39×10^{-13}	4.33×10^{-13}
14	70	1.84×10^{-8}	3.78×10^{-13}	5.31×10^{-13}	5.32×10^{-13}	5.07×10^{-13}	3.66×10^{-13}
16	135	7.74×10^{-7}	3.02×10^{-12}	3.38×10^{-12}	3.45×10^{-12}	3.59×10^{-12}	2.7×10^{-12}
18	135	3.22×10^{-6}	2.25×10^{-12}	3.36×10^{-12}	3.48×10^{-12}	3.36×10^{-12}	2.08×10^{-12}
20	231	0.000 282	1.67×10^{-11}	1.96×10^{-11}	1.98×10^{-11}	2.05×10^{-11}	1.61×10^{-11}
22	231	0.000 98	1.22×10^{-11}	1.84×10^{-11}	1.92×10^{-11}	1.76×10^{-11}	1.07×10^{-11}
24	364	0.0833	9.58×10^{-11}	1.09×10^{-10}	1.1×10^{-10}	1.09×10^{-10}	9.14×10^{-11}
26	364	0.643	6.38×10^{-11}	9.41×10^{-11}	1.05×10^{-10}	9×10^{-11}	5.72×10^{-11}
28	540	60.9	5.45×10^{-10}	6.19×10^{-10}	6.37×10^{-10}	6.11×10^{-10}	5.25×10^{-10}
30	540	124	3.28×10^{-10}	5.09×10^{-10}	5.3×10^{-10}	4.59×10^{-10}	2.93×10^{-10}
32	765	4.26×10^{4}	2.93×10^{-9}	3.35×10^{-9}	3.38×10^{-9}	3.26×10^{-9}	2.87×10^{-9}

Table 1.3: 3HOB calculation time in seconds, using different approaches for 9j symbol evaluation. E is the energy of the HO; L is equal to E/2; Dim is the dimension of matrix.

E	Dim	Bin	Wei	$TuzDir$	$TuzRec$	$WigXj6j$	$WigXj9j$
8	30	0.008	0.053	0.006	0.007	0.013	0.01
10	30	0.016	0.133	0.013	0.013	0.03	0.021
12	70	0.1	0.886	0.079	0.085	0.192	0.137
14	70	0.184	1.94	0.144	0.157	0.401	0.277
16	135	0.809	8.9	0.632	0.692	1.75	1.22
18	135	1.37	17.1	1.09	1.18	3.32	2.29
20	231	4.75	62.3	3.74	4.09	11.5	7.92
22	231	7.58	110	6.13	6.61	20.5	14
24	364	22.1	333	17.8	19.3	60.1	40.7
26	364	33.8	557	27.9	30	101	68.2
28	540	86.7	1.48×10^3	70.8	76.9	258	174
30	540	127	2.34×10^3	107	115	409	280
32	765	305	5.6×10^3	246	265	959	646

Table 1.4: Number of all 3HOB coefficients in range [0,E], where E is HO energy quanta. Num- number of coefficients

E	8	9	10	11	12	13	14	15
Num	3245	5836	10127	16784	27032	64056	94992	138225

1.5.2 The reconstruction of the 3HOB matrix

The number of HOBs required to fill the matrix grows rapidly as the dimensions of the matrices rise (tbl.(1.4)).

The dimensions of matrices depend on the total harmonic oscillator energy and the angular momenta values. The direct calculation of HOBs using the eq.(3.5) relies on the 9j symbol, the 6j symbol, and the binomial and the trinomial coefficients [47]. The computation of these coefficients is expensive and often takes a large fraction of total computing time. In many cases, HOBs evaluations can consume as much as 40 percent of the total computing time. The HOB calculations are often repetitive and require the values, which were already calculated. To reduce the recalculation to maximum, one can store the evaluated coefficients in the memory of the computer. However, the number of calculated coefficients rises very rapidly when the total HO energy quanta is increased. That makes the effective storage and retrieval of values a problem. One of the obvious solutions is to employ the symmetries of HOBs(eqs.(1.81,1.82,1.83,1.84,1.85)) to reduce the amount of values required to store. This allows using while slow, but very accurate calculation methods for initial HOB calculation. Therefore, we extend the range of the stability of the whole calculation and provide more accurate results.

Let us reintroduce the symmetries of HOBs

$$\begin{aligned}
&\langle e_1 l_1, e_2 l_2 : \Lambda \,|EL, el : \Lambda\rangle_d \\
&= \langle EL, el : \Lambda \,|e_1 l_1, e_2 l_2 : \Lambda\rangle_d && (1.92)\\
&= (-1)^{L+l_2} \langle e_2 l_2, e_1 l_1 : \Lambda \,|el, EL : \Lambda\rangle_d && (1.93)\\
&= (-1)^{\Lambda-L} \langle e_2 l_2, e_1 l_1 : \Lambda \,|EL, el : \Lambda\rangle_{1/d} && (1.94)\\
&= (-1)^{\Lambda-l_1} \langle e_1 l_1, e_2 l_2 : \Lambda \,|el, EL : \Lambda\rangle_{1/d}\,. && (1.95)
\end{aligned}$$

Which symmetry properties can be used to optimize the evaluation depends on the parameter d. If $d \neq 1$, only the symmetry properties from eqs.(1.92 - 1.93) can be used. The relations in eq.(1.94) and in eq.(1.95) are valid for reverse parity of Jacobi tree, where the d parameter is inverted ($\frac{1}{d}$). All symmetry relations can be employed for a special case when $d = 1$. By using the eq.(1.92) and eq.(1.93) we can reduce the amount of matrix elements required to calculate to the quarter of the full matrix. Additional symmetry relations eq.(1.94) and eq.(1.95) allow the additional reduction to total of $\frac{1}{8}$ of the matrix. Using this approach, not only we can reduce the amount of memory required to store matrix values, but also to speed up the calculation.
This type of approach requires to construct the symmetric numeration of matrix parameters required to evaluate the HOB matrix elements. The symmetric numeration allows separating and evaluating unique matrix values at the initial stage of calculation. It also simplifies the formation of HOB matrix by grouping the matrix values according to the symmetry relations. For identification of the stored values, the tagging algorithm was designed.

When the mass ratio parameter d is equal to 1, all the symmetry relations can be used to reconstruct the full HOB matrix. The matrix is partitioned to the structure in fig.(1.4). The partitioning is valid for even total HO energy values. At the initial stage, we need to calculate sectors α_1, β_1, γ. When the HO energy values are odd, only γ sector needs to be pre-calculated. In general, the HOB matrix values can be classified into three groups- α_1,β_1,γ, which can be referenced as the buckets. Buckets are correct for all the HO energy values with a particular mass ratio parameter d. In this case $d = 1$. By correctly tagging the matrix values, we can avoid creating multiple buckets for the range of matrices needed and create three general buckets. We tag these values by using the HOB matrix element parameters consisting of the HO energy and the angular momenta quantum numbers $e_1, l_1, e_2, l_2, e_1^{'}, l_1^{'}, e_2^{'}, l_2^{'}$. An additional HOB matrix identificator e, l is needed.

The binary tree for the tag creation process is presented in fig.(1.5). At first, we calculate pair tags:

- $t_1 = e_1 * (e_1 + 1) + l_1$-corresponding to the pair e_1, l_1

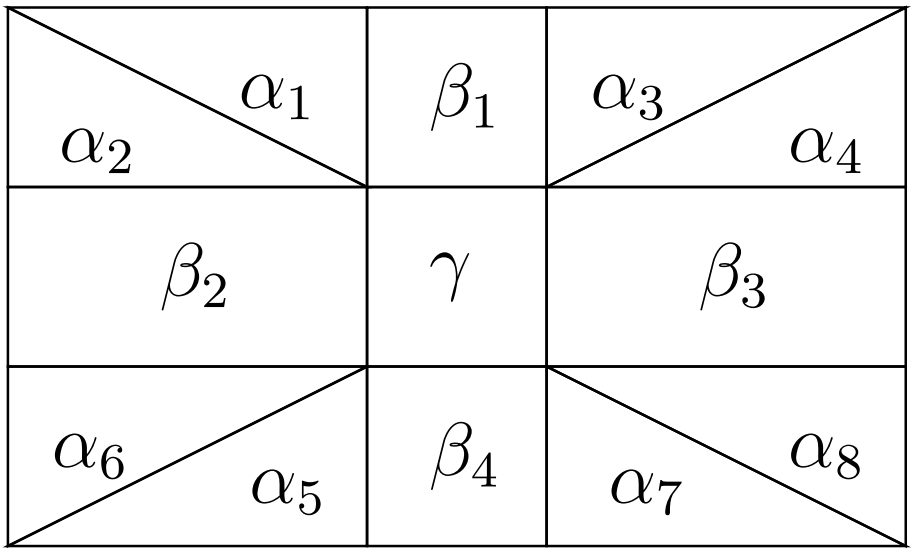


Figure 1.4: Matrix sectors

- $t_2 = e_2 * (e_2 + 1) + l_2$-corresponding to the pair e_2, l_2
- $t_1' = e_1' * (e_1' + 1) + l_1'$-corresponding to the pair $e_1^{'}, l_1^{'}$
- $t_2' = e_2' * (e_2' + 1) + l_2'$-corresponding to the pair $e_2^{'}, l_2^{'}$
- $t_t = t_1 * (t_1 + 1) + t_2$-corresponding to the pair t_1, t_2
- $t_t' = t_1' * (t_1' + 1) + t_2'$-corresponding to the pair $t_1^{'}, t_2^{'}$

Then we need to identify in which matrix sector the required value is. Also, there is a central sector (marked yellow) and already calculated values (marked green). The identification of the sector is done by splitting the matrix into three groups and subsequently identifying the sector (fig.(1.6)). The group identification is done by using tags t_1 and t_2.

- **First group**: when $t_1 > t_2$ then we have upper sectors 1, *Green*, $4^{'}$, 2, 3. The first group sector is identified following the rules:
  - $(t_1 \geq t_1') \cap (t_1' > t_2') \cap (tt \geq tt') \rightarrow$ we have *Green* sector.
  - $(t_1 \leq t_1') \cap (t_1' > t_2') \rightarrow 1$ sector.

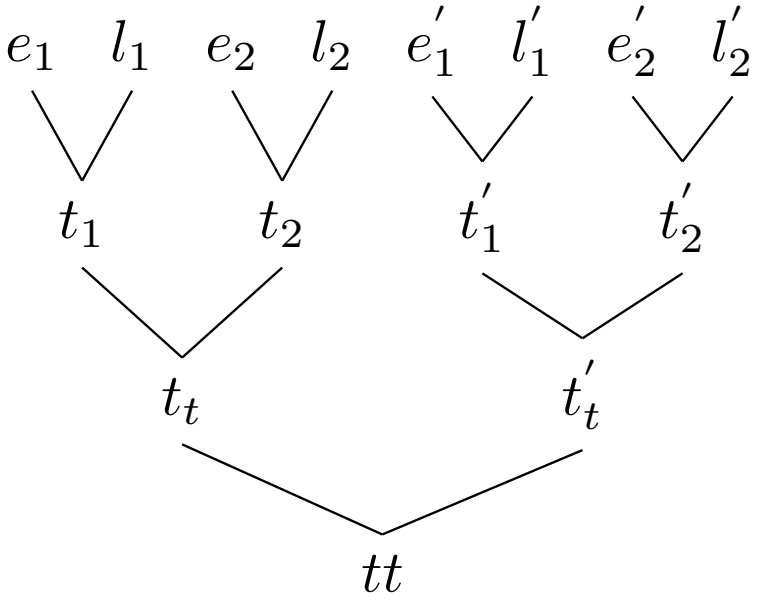


Figure 1.5: Tag formation tree

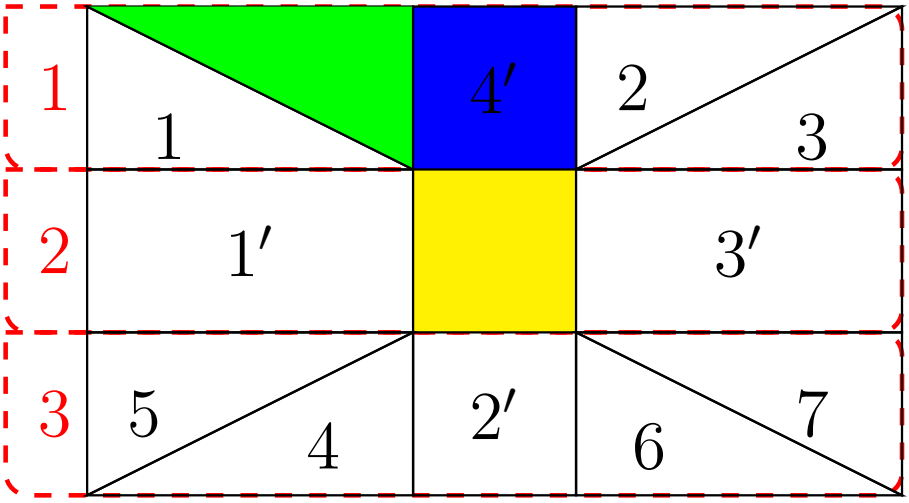


Figure 1.6: HOB matrix sector identification. Groups of sectors are identified by red numbers. Sectors are identified by numbers and colours.

- $(t_1' = t_2') \rightarrow 4^{'}$ sector.
- $(t_1 \geq t_2') \cap (tt \geq (t_2' * (t_2' + 1) + t_1')) \rightarrow 2$ sector.
- $(t_1 \leq t_2') \cap (tt \leq (t_2' * (t_2' + 1) + t_1')) \rightarrow 3$ sector.

- **Second group**: when $t_1 = t_2$ then we have middle sectors $1^{'}$,$Yellow$,$3^{'}$. The second group sector is identified following the rules:
  - $(t_1' > t_2') \rightarrow 1'$ sector.
  - $(t_1' = t_2') \rightarrow Yellow$ sector.
  - $(t_1' < t_2') \rightarrow 3'$ sector.

- **Third group**: when $t_1 < t_2$ then we have the lower matrix sectors 5, 4, $2^{'}$, 6, 7. The third group sector is identified following the rules:
  - $(t_1' \geq t_2) \cap ((t_2 * (t_2 + 1) + t_1) \leq tt') \cap (t_1' > t_2')) \rightarrow 5$ sector.
  - $(t_2 \geq t_1') \cap (t_1' > t_2') \rightarrow 4$ sector.
  - $(t_1' = t_2') \rightarrow 2^{'}$ sector.
  - $(t_2 \geq t_2') \cap ((t_2 * (t_2 + 1) + t_1) \geq (t_2' * (t_2' + 1) + t_1')) \rightarrow 6$ sector
  - $(t_2' = t_2) \rightarrow$sector.

After locating the sector, the suitable phase multiplier can be calculated. Then it can be determined in which bucket the required value is located. The phase multiplier is calculated according to symmetry rules and the retrieved value is multiplied by it. When the sector is determined it becomes possible to calculate the hash identifier of the value.

Hashing

The identifier or the *hash* of the value is computed using the values e, l for matrix identification and t_1, t_2, $t_1^{'}$, $t_2^{'}$ for the value identification. Values t_1, t_2, $t_1^{'}$, $t_2^{'}$ are composed in the specific order to reflect in which sector the value is located. The tag is the prime number.

One can use any hashing algorithm which is faster than the calculation of the coefficients and does not produce collisions. When the tag is calculated, the value is looked up in the corresponding bucket.

This algorithm allows the retrieval of the desired value faster than direct calculation. The required value can be calculated during the program execution and put in the bucket for later use. This eliminates the need to store the whole matrix values. Moreover, not all matrix values could be needed for the calculation of the operators. The drawback of this approach is that the bucket is not sorted thus disallowing the use of the faster search algorithm (e.g. various implementations of the binary search tree).

A test was performed of such an approach in the calculation of 3HOB matrix. The time of the calculation of the full matrix with $d = 1$ was compared with the time of the reconstructed matrices from $\frac{1}{4}$ and $\frac{1}{8}$ of the whole matrix. The results are presented in the tbl.(1.5). They show that this approach is very useful for matrix construction as it allows the speedup of the calculation up to 725 percent.

Table 1.5: The Standard 3HOB matrix calculation vs reconstruction. E is the HO energy; L is the angular momenta; Dim is the Dimension of the matrix; Full is full matrix calculation without the symmetries; $\frac{1}{4}$ is time of matrix reconstruction using the symmetries, reconstructing from fourth of the whole matrix; $\frac{1}{8}$ is the time of reconstruction from the eight of the matrix; Speedups show how faster we can get the same matrix from reconstruction compared to the full matrix calculation in percentage.

E	L	Dim	$Full$	$\frac{1}{4}$	$\frac{1}{8}$	$Speedup(\frac{1}{4})\%$	$Speedup(\frac{1}{8})\%$
12	6	70	0.27	0.11	0.03	246	733
14	7	70	0.48	0.16	0.07	286	688
16	8	135	2.15	0.68	0.3	313	707
18	9	135	3.78	1.13	0.53	330	691
20	10	231	12.88	3.76	1.77	342	721
22	11	231	21	6.08	2.97	345	705
24	12	364	60	17.1	8.3	354	725

Chapter 2

Six nucleon system in Jacobi coordinates

To explore the six body systems using the formalism introduced in chapter 1 one has to construct the coefficients of fractional parentage (CFPs). Depending on the chosen Jacobi coordinates and the structure of the Jacobi tree one can use the binary cluster formalism. Firstly, we construct the CFPs for the subclusters and then for the whole system.

Let us consider a structure of the six nucleon system composed of clusters consisting of three nucleons. For the calculations, we employ the Λ operator formalism and follow the operator P_{1N_1+1}. The three-particle subclusters are partitioned into $1 + 2$ system. For the Λ operator construction, the operator P_{13} of the symmetric group S_3 is chosen. When we calculate the CFPs for the subclusters we can construct the CFPs for the whole system. To construct the six particle Λ operator the transposition operator P_{14} of the symmetric group S_6 is chosen.

2.1 The CFPs of the three-nucleon subcluster

In this section, the construction of the CFPs for the three-nucleon subclusters of the six nucleon system is considered. In the CFP formalism we partition the six nucleon system into the two three-body

clusters and find the antisymmetric subspaces for these subclusters. Only then the full antisymmetric subspace can be found.

One starts by introducing the Jacobi tree for the three particles (fig.(2.1)).

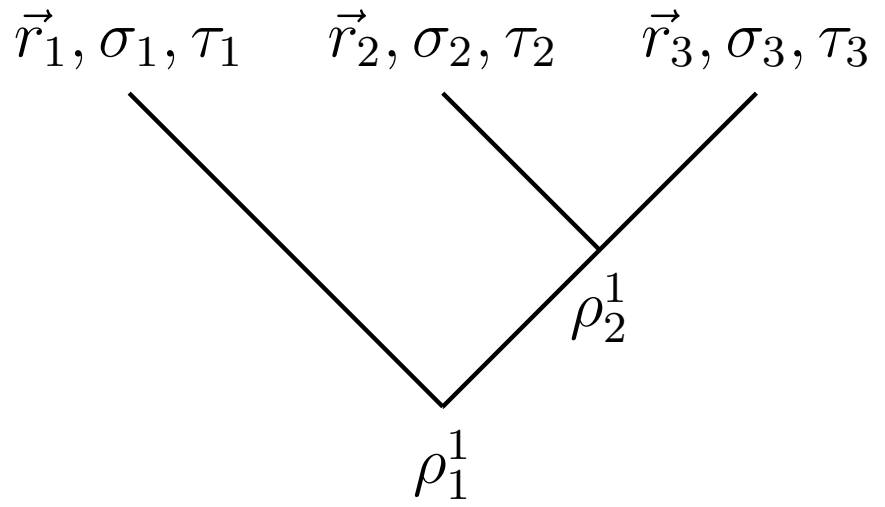


Figure 2.1: Jacobi tree for three-particle system. ρ_y^x is the Jacobi coordinate, where the x is cluster number, y is the coordinate number, r- particle coordinate,σ - the particle spin coordinate, τ - is the particle isospin coordinate.

This Jacobi tree corresponds to the following Jacobi coordinates

$$\boldsymbol{\rho}_1^1 = \sqrt{\frac{2}{3}}(\boldsymbol{r}_1 - \frac{1}{2}(\boldsymbol{r}_2 + \boldsymbol{r}_3)), \tag{2.1}$$
$$\boldsymbol{\rho}_2^1 = \frac{1}{\sqrt{2}}(\boldsymbol{r}_2 - \boldsymbol{r}_3).$$

Since the c.m. coordinate does not change in any kind of the permutations is not included. $\boldsymbol{\rho}_2^1$ coordinate couples the second and third nucleons. The coordinate $\boldsymbol{\rho}_1^1$ couples the first nucleon to the second and third. These are the coordinates corresponding to the first subcluster of the system. For the presented coordinates the corresponding basis vectors in the HO basis can be denoted as

$$|((e_1 l_1, \frac{1}{2})j_1, \left(\overline{E}_1 \overline{L}_1, \overline{S}_1\right) \overline{J}_1); (\frac{1}{2}, \overline{T}) \left[1^2\right]) E_1 J_1 T_1\rangle \qquad (2.2)$$

Here $e_1 l_1$ and $\overline{E}_1 \overline{L}_1$ are the HO excitation energy and the corresponding angular momenta quantum numbers. They correspond to the harmonic oscillators associated with the coordinates $\boldsymbol{\rho}_1^1$ and $\boldsymbol{\rho}_2^1$ respectively. Quantum numbers $\overline{S}_1, \overline{T}_1, \overline{J}_1$ describe the spin, isospin, and the total angular momentum of the relative-coordinate two-nucleon channel. The quantum number j_1 is the total angular momentum of the first nucleon relative to the center of mass of the nucleons 2 and 3. The quantum numbers J_1 and T_1 are the total angular momentum and the total isospin of the first cluster, respectively. The basis vector in eq.(2.2) is antisymmetric with respect of the nucleons 2 and 3. These two-nucleon channel quantum numbers are restricted by the condition $(-1)^{\overline{L}_1+\overline{S}_1+\overline{T}_1} = -1$. If this condition is satisfied then the two nucleon space is automatically restricted to the antisymmetric subspace. The Young Diagram representation of the antisymmetric two nucleon system is $\left[1^2\right]$. However it is not antisymmetric with the respect to the exchanges of the nucleon 1 with the nucleons 2 and 3.. To construct an antisymmetric subspace, the operator Λ of the symmetric group S_3 will be used. The Λ operator for the Jacobi tree presented in fig.(2.1) is

$$\Lambda_3(\lambda) = \overline{\Lambda}_1\left(\left[1^2\right]\right) + P_{12} + P_{13} = \overline{\Lambda}_1\left(\left[1^2\right]\right) + 2P_{13}. \qquad (2.3)$$

Then the calculation of the Λ operator for the three-nucleon system is

$$P_{13} = \frac{1}{2}(\Lambda(\lambda) - \overline{\Lambda}_1\left(\left[1^2\right]\right)). \qquad (2.4)$$

For the acquisition of the CFPs one has to obtain the eigenvectors of the operator P_{13}. The matrix element for the operator P_{13} in the HO basis is calculated in a pretty straightforward way by using the angular momenta recoupling coefficient notation presented in subsection 1.4.1

$$\begin{aligned}
&\langle(((e_1 l_1, \frac{1}{2}) j_1, (\overline{E_1 L_1}, \overline{S}_1)\overline{J}_1); (\frac{1}{2}, \overline{T}_1)\,[1^2])E_1 J_1 T_1 | P_{13} \times \\
&\quad |(((e_1' l_1', \frac{1}{2}) j_1', (\overline{E}_1' \overline{L}_1', \overline{S}_1')\overline{J}_1'); (\frac{1}{2}, \overline{T}_1')\,[1^2])E_1 J_1 T_1\rangle \\
&\qquad = (-1)^{L+\overline{L}'+\overline{S}+\overline{S}'+\overline{T}+\overline{T}'} \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \overline{T}_1' \\ \frac{1}{2} & \overline{T}_1 & T \end{bmatrix} \qquad (2.5) \\
\times \sum_{LS} (-1)^L &\begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \overline{S}_1' \\ \frac{1}{2} & \overline{S}_1 & S \end{bmatrix} \begin{bmatrix} l_1 & \overline{L}_1 & L \\ \frac{1}{2} & \overline{S_1} & S \\ j_1 & \overline{J}_1 & J \end{bmatrix} \begin{bmatrix} l_1' & \overline{L}_1' & L \\ \frac{1}{2} & \overline{S}_1' & S \\ j' & \overline{J}_1' & J \end{bmatrix} \\
&\times \langle e_1 l_1, \overline{E}_1 \overline{L}_1 : L | \overline{E}_1' \overline{L}_1', e_1' l_1' : L\rangle_3.
\end{aligned}$$

The bracket $\langle e_1 l_1, \overline{E}_1 \overline{L}_1 : L | \overline{E}_1' \overline{L}_1', e_1' l_1' : L\rangle_3$ is the general harmonic oscillator bracket with a mass-ratio parameter $d = 3$ [60]. The quantum numbers $e_1 l_1 j_1$ are the harmonic oscillator (HO) energy, angular momentum, and the total angular momentum corresponding to the Jacobi coordinate $\boldsymbol{\rho}_1^1$. The quantum numbers $\overline{E}_1 \overline{L}_1 \overline{S}_1 \overline{J}_1 \overline{T}_1$ are the HO energy, angular momentum, total angular momentum, spin, and isospin corresponding to the Jacobi coordinate $\boldsymbol{\rho}_2^1$. The quantum numbers $e_1' l_1' j_1'$ and $\overline{E}_1' \overline{L}_1' \overline{S}_1' \overline{J}_1' \overline{T}_1'$ are the same quantities, corresponding to the transformed Jacobi coordinates $\boldsymbol{\rho}_1^{1'} = \sqrt{\frac{2}{3}}(\boldsymbol{r}_3 - \frac{1}{2}(\boldsymbol{r}_2 + \boldsymbol{r}_1))$ and $\boldsymbol{\rho}_2^{1'} = \frac{1}{\sqrt{2}}(\boldsymbol{r}_2 - \boldsymbol{r}_1)$. The quantum numbers L and S are the total angular momentum and the total spin. The total oscillator energy, total angular momentum and the isospin of the three-nucleon system are denoted as $E_1 J_1 T_1$.

We denote the antisymmetric three-nucleon state vectors as $|EJT\Delta\,[1^3]\rangle$. $[1^3]$ is the Young diagram of the antisymmetric subspace for three particles. Δ is an additional quantum number for the enumeration of the states with the same set of quantum numbers in the $[1^3]$ subspace [61]. The completely antisymmetric state vectors $|EJT\Delta\,[1^3]\rangle$ are expanded in terms of the complete set of coupled parent state vectors with a lower degree of antisymmetry:

$$|EJT\Delta\left[1^3\right]\rangle = \sum_{e_1 l_1 j_1 \overline{E}_1 \overline{L}_1 \overline{S}_1 \overline{J}_1 \overline{T}_1} |(((e_1 l_1, \frac{1}{2}) j_1, (\overline{E}_1 \overline{L}_1, \overline{S}_1)\overline{J}_1); (\frac{1}{2}, \overline{T}_1)\left[1^2\right]) EJT\rangle \tag{2.6}$$
$$\times \langle (((e_1 l_1, \frac{1}{2}) j_1, (\overline{E}_1 \overline{L}_1, \overline{S}_1)\overline{J}_1); (\frac{1}{2}, \overline{T}_1)\left[1^2\right]) EJT | EJT\Delta\left[1^3\right]\rangle.$$

$|e_1 l_1 j_1\rangle$ and $\left|\overline{E}_1 \overline{L}_1 \overline{S}_1 \overline{T}_1 \left[1^2\right]\right\rangle$ are the state vectors of the one and two nucleon clusters. The expansion coefficients

$$\langle (((e_1 l_1, \frac{1}{2}) j_1, (\overline{EL}, \overline{S})\overline{J}); (\frac{1}{2}, \overline{T})\left[1^2\right]) EJT | EJT\Delta\left[1^3\right]\rangle \tag{2.7}$$

are the CFPs for the three-particle system. For the CFP calculation in the three-nucleon case, it is enough to calculate the matrix of the operator P_{13}. The eigenvalues of the operator P_{13} and the corresponding Young diagrams were described in subsection 1.3.4. The eigenvectors of the operator P_{13}, corresponding to the eigenvalue -1, are CFPs of the three-nucleon system. The same procedure must be applied for the second subcluster as well.

2.2 The CFPs for the six nucleon system

2.2.1 Jacobi coordinates and the Λ operator

In this subsection, the construction of the antisymmetrized state vectors for the six nucleon system is presented. When one has two antisymmetrized subclusters consisting of three nucleons, the construction of the antisymmetric state vectors for the whole system is relatively straightforward, although it requires meticulous work with the angular momenta algebra. We start by introducing the Jacobi coordinates for the six nucleon system

$$
\begin{aligned}
\rho_1^1 &= \sqrt{\frac{2}{3}}(\boldsymbol{r}_1 - \frac{1}{2}(\boldsymbol{r}_2 + \boldsymbol{r}_3)),\\
\rho_2^1 &= \frac{1}{\sqrt{2}}(\boldsymbol{r}_2 - \boldsymbol{r}_3),\\
\rho_1^2 &= \sqrt{\frac{2}{3}}(\boldsymbol{r}_4 - \frac{1}{2}(\boldsymbol{r}_5 + \boldsymbol{r}_6)),\\
\rho_2^2 &= \frac{1}{\sqrt{2}}(\boldsymbol{r}_5 - \boldsymbol{r}_6),\\
\rho_r &= \frac{1}{\sqrt{6}}(\boldsymbol{r}_1 + \boldsymbol{r}_2 + \boldsymbol{r}_3 - \boldsymbol{r}_4 - \boldsymbol{r}_5 - \boldsymbol{r}_6).
\end{aligned}
\tag{2.8}
$$

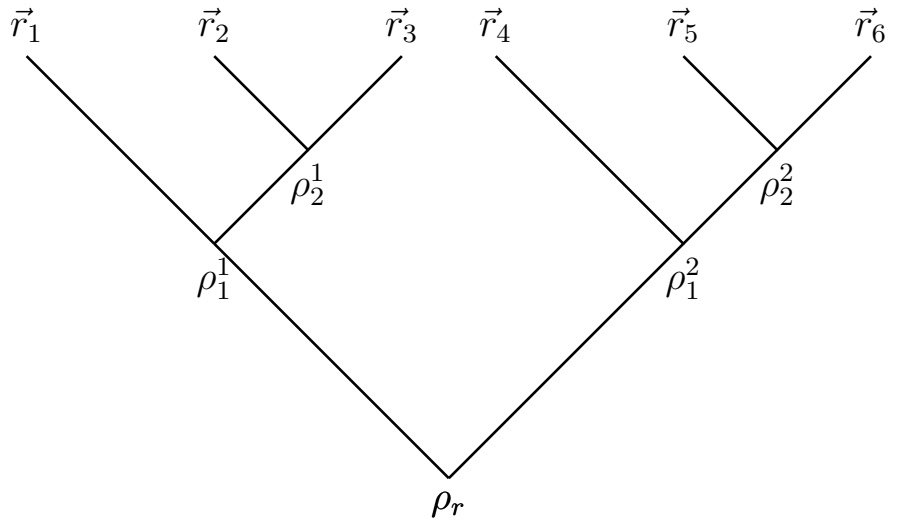
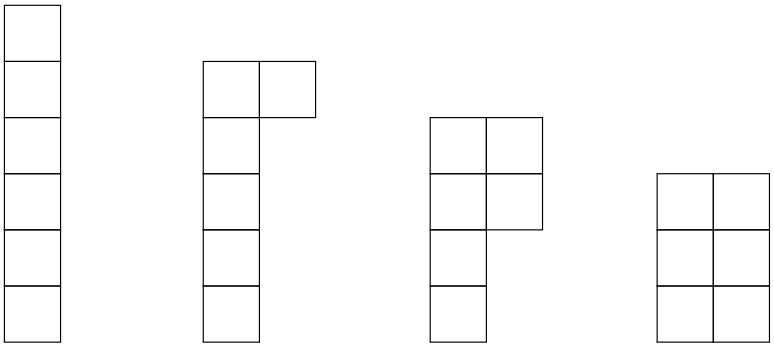


Figure 2.2: Jacobi tree for six nucleon system. ρ_y^x is the Jacobi coordinate, where the x is cluster number, y is the coordinate number, r-particle coordinate.

The Jacobi tree for the coordinates from eq.(2.8) is presented in fig.(2.2). The set of coordinates ρ_1^1, ρ_2^1 and ρ_1^2, ρ_2^2 describe the motion inside the first and the second subclusters of the system respectively. The coordinate ρ_r denotes the relative motion between these subclusters. The HO state vectors for the six nucleon system



$a)[\lambda_1] = [1^6]$ $b)[\lambda_2] = [21^4]$ $c)[\lambda_3] = [2^2 1^2]$ $d)[\lambda_4] = [2^3]$

Figure 2.3: The Young Diagrams for the four configurations of irreps produced from the two antisymmetric subspaces of the three-particle subclusters. a) corresponds to the fully antisymmetric one $[1^6]$. Other configurations have lesser degree of antisymmetry.

in the antisymmetric three-particle cluster subspaces are equal to

$$|\left(\left(\left(E_1 J_1 T_1 \Delta_1 \left[1^3\right]\right), \left(E_2 J_2 T_2 \Delta_2 \left[1^3\right]\right) \overline{J} T_6\right); e_r l_r\right) E_6 J_6 T_6\rangle. \quad (2.9)$$

Here $E_i J_i T_i \Delta_i \left[1^3\right]$ $i = 1, 2$ are the quantum numbers of three-nucleon systems, described in eq.(2.6). $e_r l_r$ is the HO energy, and the angular momentum corresponding to the relative motion coordinate ρ_r. $\overline{J}$ denotes the intermediate angular momentum. The quantum numbers $E_6 J_6 T_6$ are the total HO energy, the total angular momentum, and the total isospin of the six nucleon system.

From the antisymmetric irreps $[1^3]$ from each subclusters, we get four possible irrep configurations: the fully antisymmetric one -$[1^3]$ and irreps with a lesser degree of antisymmetry- $[21^4]$, $[2^3]$ and $[2^2 1^2]$ (fig.(2.3)).

The antisymmetric angular momentum coupled six nucleon state vectors $|E_6 J_6 T_6 \Delta_6 \left[1^6\right]\rangle$ are expanded in the terms of the two antisymmetrical three-nucleon state vectors

$$\begin{aligned}\left|E_6 J_6 T_6 \Delta_6 \left[1^6\right] \left[1^3\right] \left[1^3\right]\right\rangle = \\ \sum_{\substack{E_1 J_1 T_1 \Delta_1 E_2 \\ J_2 T_2 \Delta_2 \overline{J} e_r l_r}} \left|\left(\left(E_1 J_1 T_1 \Delta_1, E_2 J_2 T_2 \Delta_2\right)\overline{J}, e_r l_r\right) E_6 J_6 T_6 \left[1^3\right] \left[1^3\right]\right\rangle \\ \times\left\langle\left(\left(E_1 J_1 T_1 \Delta_1, E_2 J_2 T_2 \Delta_2\right)\overline{J}, el\right) E_6 J_6 T_6 \left[1^3\right] \left[1^3\right]\right. \\ \left.\times\left|E_6 J_6 T_6 \Delta_6 \left[1^6\right] \left[1^3\right] \left[1^3\right]\right\rangle.\end{aligned} \tag{2.10}$$

Like in the three-nucleon case, the expansion coefficients

$$\left\langle\left(\left(E_1 J_1 T_1 \Delta_1, E_2 J_2 T_2 \Delta_2\right)\overline{J}, el\right) E_6 J_6 T_6 \left[1^3\right] \left[1^3\right] \left|E_6 J_6 T_6 \Delta_6 \left[1^6\right] \left[1^3\right] \left[1^3\right]\right\rangle \tag{2.11}$$

are the CFPs of the first and the second three-nucleon clusters. Following the formalism introduced in subsection 1.3.4 we will construct the Λ_6 operator.

$$\begin{aligned}\Lambda_6(\lambda) &= \overline{\Lambda}_1\left(\left[1^3\right]\right) + \overline{\Lambda}_2\left(\left[1^3\right]\right) + \sum_{r=1}^{3}\sum_{q=6-3+1}^{6} P_{rq} \\ &= \overline{\Lambda}_1\left(\left[1^3\right]\right) + \overline{\Lambda}_2\left(\left[1^3\right]\right) + 9P_{14}.\end{aligned} \tag{2.12}$$

For the operator P_{rq} following the nomenclature of the operator P_{1N_1+1} we will choose the two-body permutation operator P_{14} of the symmetric group S_6. The permutation operator P_{14} consists of three components, namely, orbital- r, spin- σ and the isospin- τ. Orbital and spin quantum numbers L and S are coupled to produce the total angular momentum J. The isospin part is not coupled to the other parts. As a result, the operator P_{14} can be expressed as a product of the matrix elements of two operators:

$$\left\langle P_{14}\right\rangle = \left\langle P_{14}^{\sigma r}\right\rangle \left\langle P_{14}^{\tau}\right\rangle. \tag{2.13}$$

The operator P_{14}^{τ} acts upon the isospin variables and the operator $P_{14}^{\sigma r}$ acts upon the spin-orbital part of the state vectors. The representation of the P_{14}^{τ} matrix element is identical to the P_{14}^{σ}.

2.2.2 The action of P_{14} on the spin

The operator P_{14}^{σ} can be calculated relatively easily. We start by introducing the basis vector for the spin

$$\left|((s_1,\overline{S}_1)S_{\,1},(s_2,\overline{S}_2)S_{\,2})S_{12}\right\rangle . \tag{2.14}$$

Here the s_x are the quantum numbers of the first coordinate of the cluster number x, while the quantum numbers $\overline{S}_x$ are related to the second coordinate of the cluster number x. The quantum number denoted as the S_x is the total spin of the respective cluster. Both clusters are coupled using the angular momenta algebra into the total system spin S_{12}. For the calculation of P^{σ}_{14} we must recouple the basis vector $\left|((s_1,\overline{S}_1)S_{\,1},(s_2,\overline{S}_2)S_{\,2})S_{12}\right\rangle$ to $\left|((s_1,s_2)s_{12},(\overline{S}_1,\overline{S}_2)\overline{S}_{12})S_{12}\right\rangle$ using the angular momenta algebra technique. We use the square angular momenta recoupling brackets

$$\left|((s_1,\overline{S}_1)S_{\,1},(s_2,\overline{S}_2)S_{\,2})S_{12}\right\rangle = \sum_{s_{12}\overline{S}_{12}} \left|((s_1,s_2)s_{12},(\overline{S}_1,\overline{S}_2)\overline{S}_{12})S_{12}\right\rangle \begin{bmatrix} s_1 & s_2 & s_{12} \\ \overline{S}_1 & \overline{S}_2 & \overline{S}_{12} \\ S_1 & S_2 & S_{12} \end{bmatrix} \delta_{\delta_{\overline{S}_1\overline{S}_2\overline{S}_{12}S_{12}}}. \tag{2.15}$$

The operator action is equal to $(-1)^{s'_1+s'_2-s'_{12}}$ and then the recoupling to the original basis vector $\left|((s_1,\overline{S}_1)S_{\,1},(s_2,\overline{S}_2)S_{\,2})S_{12}\right\rangle$ must follow. The final expression for the P^{σ}_{14} matrix element is equal to

$$\left\langle((s_1,\overline{S}_1)S_{\,1},(s_2,\overline{S}_2)S_{\,2})S_{12}\right| P^{\sigma}_{14} \left|((s_1,\overline{S}_1)S'_{\,1},(s_2,\overline{S}_2)S'_{2})S_{12}\right\rangle = \sum_{s_{12}\overline{S}_{12}} \begin{bmatrix} s_1 & \overline{S}_1 & S_1 \\ s_2 & \overline{S}_2 & S_2 \\ s_{12} & \overline{S}_{12} & S_{12} \end{bmatrix} (-1)^{s_1+s_2-s_{12}} \begin{bmatrix} s_1 & s_2 & s_{12} \\ \overline{S}_1 & \overline{S}_2 & \overline{S}_{12} \\ S'_1 & S'_2 & S_{12} \end{bmatrix} \tag{2.16}$$

$$\times\delta_{s_1s_2s_{12}\overline{S}_1\overline{S}_2\overline{S}_{12}S_{12},s'_1s'_2s'_{12}\overline{S}'_1\overline{S}'_2\overline{S}'_{12}S'_{12}}. \tag{2.17}$$

This expression can is simplified using the properties of the 9j coefficients. By going from the RECs to the 9j symbols, we can exploit the symmetries of these symbols and sum up the two 9j symbols into one. Firstly, we rewrite the recoupling coefficients from the quadratic brackets into the full expressions with the 9j symbols and corresponding dimensional multipliers

$$\left\langle((s_1,\overline{S}_1)S\,_1,(s_2,\overline{S}_2)S\,_2)S_{12}\right|P_{14}^{\sigma}\left|((s_1,\overline{S}_1)S'\,_1,(s_2,\overline{S}_2)S'\,_2)S'_{12}\right\rangle\delta_{S_{12}S'_{12}}=$$
$$\sum_{s_{12}\overline{S}_{12}}\begin{bmatrix} s_1 & \overline{S}_1 & S_1 \\ s_2 & \overline{S}_2 & S_2 \\ s_{12} & \overline{S}_{12} & S_{12}\end{bmatrix}(-1)^{s_1+s_2-s_{12}}\begin{bmatrix} s_1 & s_2 & s_{12} \\ \overline{S}_1 & \overline{S}_2 & \overline{S}_{12} \\ S'_1 & S'_2 & S_{12}\end{bmatrix} \tag{2.18}$$
$$\times\delta_{s_1s_2\overline{S}_1\overline{S}_2\overline{S}_{12}S_{12},s'_1s'_2\overline{S}'_1\overline{S}'_2\overline{S}'_{12}S'_{12}}$$
$$=\sum_{s_{12}\overline{S}_{12}}\sqrt{d_{s_{12}}d_{\overline{S}_{12}}d_{S_1}d_{S_2}}\sqrt{d_{s'_{12}}d_{\overline{S}_{12}}d_{S'_1}d_{S'_2}}$$
$$\times\begin{Bmatrix} s_1 & \overline{S}_1 & S_1 \\ s_2 & \overline{S}_2 & S_2 \\ s_{12} & \overline{S}_{12} & S_{12}\end{Bmatrix}(-1)^{s'_1+s'_2-s'_{12}}\begin{Bmatrix} s_2 & s_1 & s_{12} \\ \overline{S}_1 & \overline{S}_2 & \overline{S}_{12} \\ S'_1 & S'_2 & S_{12}\end{Bmatrix}.$$

Some of the dimensional multipliers and phasis multipliers can be transferred outside of the sum as they are independent of the summation. Also one must account for the delta functions in eq.(2.18). The resulting equation is

$$(-1)^{s_1+s_2}\sqrt{d_{S_1}d_{S_2}d_{S'_1}d_{S'_2}}\sum_{s_{12}\overline{S}_{12}}d_{s_{12}}d_{\overline{S}_{12}} \tag{2.19}$$
$$\times\begin{Bmatrix} s_1 & \overline{S}_1 & S_1 \\ s_2 & \overline{S}_2 & S_2 \\ s_{12} & \overline{S}_{12} & S_{12}\end{Bmatrix}(-1)^{s_{12}}\begin{Bmatrix} s_2 & s_1 & s_{12} \\ \overline{S}_1 & \overline{S}_2 & \overline{S}_{12} \\ S'_1 & S'_2 & S_{12}\end{Bmatrix}.$$

The next step is done by using the symmetry features of the 9j symbol. The 9j symbol structure is changed and this yields an additional phase multiplier. This operation results in the equation

$$=(-1)^{s_1+s_2}\sqrt{d_{S_1}d_{S_2}d_{S'_1}d_{S'_2}} \tag{2.20}$$
$$\times\sum_{s_{12}\overline{S}_{12}}d_{s_{12}}d_{\overline{S}_{12}}(-1)^{s_1+s_2+s_{12}+\overline{S}_1+\overline{S_2}+\overline{S}_{12}+S_1+S_2+S_{12}}$$
$$\times(-1)^{s_1+s_2+s_{12}+\overline{S}_1+\overline{S_2}+\overline{S}_{12}+S'_1+S'_2+S_{12}}$$
$$\times\begin{Bmatrix} \overline{S}_1 & \overline{S}_2 & \overline{S}_{12} \\ s_1 & s_2 & s_{12} \\ S_1 & S_2 & S_{12}\end{Bmatrix}(-1)^{s_{12}}\begin{Bmatrix} \overline{S}_1 & \overline{S}_2 & \overline{S}_{12} \\ s_2 & s_1 & s_{12} \\ S'_1 & S'_2 & S_{12}\end{Bmatrix}.$$

The eq.(2.20) can be simplified by summing the two 9j symbols into one. By using the equation

$$\sum_{XY}(-1)^{Y} d_X d_Y \left\{ \begin{array}{ccc} a & b & X \\ c & d & Y \\ e & f & j \end{array} \right\} \left\{ \begin{array}{ccc} a & b & X \\ d & c & Y \\ g & h & j \end{array} \right\} = (-1)^{2b+f+h} \left\{ \begin{array}{ccc} a & d & g \\ c & b & h \\ e & f & j \end{array} \right\} \tag{2.21}$$

from [46] we get the equation

$$\begin{aligned} &= (-1)^{s_1+s_2}(-1)^{S_1+S_2}(-1)^{S_1'+S_2'}\sqrt{d_{S_1} d_{S_2} d_{S_1'} d_{S_2'}} \qquad (2.22)\\ &\times \sum_{s_{12}\overline{S}_{12}} d_{s_{12}} d_{\overline{S}_{12}} \left\{ \begin{array}{ccc} \overline{S}_1 & \overline{S}_2 & \overline{S}_{12} \\ s_1 & s_2 & s_{12} \\ S_1 & S_2 & S_{12} \end{array} \right\} (-1)^{s_{12}} \left\{ \begin{array}{ccc} \overline{S}_1 & \overline{S}_2 & \overline{S}_{12} \\ s_2 & s_1 & s_{12} \\ S_1' & S_2' & S_{12} \end{array} \right\} \\ &= (-1)^{s_1+s_2}(-1)^{S_1+S_2}(-1)^{S_1'+S_2'}\sqrt{d_{S_1} d_{S_2} d_{S_1'} d_{S_2'}}(-1)^{2\overline{S}_2+S_2+S_2'} \\ &\times \left\{ \begin{array}{ccc} \overline{S}_1 & s_2 & S_1' \\ s_1 & \overline{S}_2 & S_2' \\ S_1 & S_2 & S_{12} \end{array} \right\}. \end{aligned}$$

The next step is to restore the square brackets in the previous equation

$$\begin{aligned} &= (-1)^{s_1+s_2}(-1)^{S_1}(-1)^{S_1'}\sqrt{d_{S_1} d_{S_2} d_{S_1'} d_{S_2'}} \left\{ \begin{array}{ccc} \overline{S}_1 & s_2 & S_1' \\ s_1 & \overline{S}_2 & S_2' \\ S_1 & S_2 & S_{12} \end{array} \right\} \qquad (2.23)\\ &= (-1)^{S_1+S_1'} \left[\begin{array}{ccc} \overline{S}_1 & \frac{1}{2} & S_1' \\ \frac{1}{2} & \overline{S}_2 & S_2' \\ S_1 & S_2 & S_{12} \end{array} \right]. \end{aligned}$$

The final expression for spin part of the P_{14} is

$$\left\langle((s_1,\overline{S}_1)S\,_1,(s_2,\overline{S}_2)S\,_2)S_{12}\right|P_{14}^{\sigma}\left|((s_1',\overline{S}_1)S'\,_1,(s_2',\overline{S}_2)S'\,_2)S_{12}\right\rangle \tag{2.24}$$
$$=(-1)^{S_1+S_1'}\begin{bmatrix}\overline{S}_1 & \frac{1}{2} & S_1'\\ \frac{1}{2} & \overline{S}_2 & S_2'\\ S_1' & S_2 & S_{12}\end{bmatrix}.$$

The calculation of the matrix element for the isospin part of the operator P_{14} follows the same path.

2.2.3 The $L-S$ decoupling

The key difference is that to calculate for the spin part, one has to do the explicit spin-orbit LS decoupling. For this separation to be done the angular momenta algebra is used once again. We start by writing the spin-orbital basis vector for the six particle system

$$\left|(l_r,((((l_1,s_1)j_1,(\overline{L}_1,\overline{S}_1)\overline{J}_1)J_1,((l_2,s_2)j_2,(\overline{L}_2,\overline{S}_2)\overline{J}_2)J_2)J_{12})J\right\rangle. \tag{2.25}$$

The quantum numbers J_x represent the total momentum of the subcluster, where x is the number of the cluster. The quantum number in the form of $\overline{Y}_x$ represents the Jacobi coordinate of the two particles. The quantum numbers y_x represent the one particle variables. The relative motion of the two clusters is denoted as l_r. The HO energy quantum numbers are omitted for clarity, though they follow the same notation.

The decoupling of the orbital and the spin part of the operator P_{14} needs eight RECs which are summed over the intermediate variables. The intermediate variables are responsible for the systems total L and S couplings.

$$\left\langle (l_r,((((l_1,s_1)j_1,(\overline{L}_1,\overline{S}_1)\overline{J}_1)J_1,((l_2,s_2)j_2,(\overline{L}_2,\overline{S}_2)\overline{J}_2)J_2)J_{12})J\right| P_{14}^{r\sigma} \tag{2.26}$$

$$\times \left|(l'_r,((((l'_1,s'_1)j'_1,(\overline{L}'_1,\overline{S}'_1)\overline{J}'_1)J'_1,((l'_2,s'_2)j'_2,(\overline{L}'_2,\overline{S}'_2)\overline{J}'_2)J'_2)J'_{12})J\right\rangle$$

$$= \sum_{\substack{L_1S_1\\L_2S_2\\L_{12}S_{12}\\L}} \sum_{\substack{L'_1S'_1\\L'_2S'_2\\L'_{12}S'_{12}\\L'}} \begin{bmatrix} l_1 & s_1 & j_1 \\ \overline{L}_1 & \overline{S}_1 & \overline{J}_1 \\ L_1 & S_1 & J_1 \end{bmatrix} \begin{bmatrix} l_2 & s_2 & j_2 \\ \overline{L}_2 & \overline{S}_2 & \overline{J}_2 \\ L_2 & S_2 & J_2 \end{bmatrix}$$

$$\times \begin{bmatrix} L_1 & S_1 & J_1 \\ L_2 & S_2 & J_2 \\ L_{12} & S & J_{12} \end{bmatrix} \begin{bmatrix} L_{12} & S & J_{12} \\ l_r & 0 & l_r \\ L & S & J \end{bmatrix}$$

$$\times \left\langle ((l_1,\overline{L})L_1,(l_2,\overline{L}_2)L_2)L_{12},l_r)L\,|P_{14}^r|\,((l'_1,\overline{L}')L'_1,(l'_2,\overline{L}'_2)L'_2)L'_{12},l'_r)L\right\rangle$$

$$\times \left\langle ((s_1,\overline{S}_1)S\,_1,(s_2,\overline{S}_2)S\,_2)S\,|P_{14}^\sigma|\,((s'_1,\overline{S}'_1)S'\,_1,(s'_2,\overline{S}'_2)S'\,_2)S\right\rangle$$

$$\times \delta_{\overline{L}_1\overline{L}_2,\overline{L}'_1\overline{L}'_2};\delta_{\overline{S}_1\overline{S}_2,\overline{S}'_1\overline{S}'_2};\delta_{\overline{J}_1\overline{J}_2J,\overline{J}'_1\overline{J}'_2J'}\delta_{LS,L'S'}$$

$$\times \begin{bmatrix} L'_{12} & l'_r & L' \\ S' & 0 & S' \\ J'_{12} & l'_r & J \end{bmatrix} \begin{bmatrix} L'_1 & L'_2 & L'_{12} \\ S'_1 & S'_2 & S' \\ J'_1 & J'_2 & J'_{12} \end{bmatrix} \begin{bmatrix} l'_1 & \overline{L}'_1 & L'_1 \\ s'_1 & \overline{S}'_1 & S'_1 \\ j'_1 & \overline{J}'_1 & J'_1 \end{bmatrix} \begin{bmatrix} l'_2 & \overline{L}'_2 & L'_2 \\ s'_2 & \overline{S}'_2 & S'_2 \\ j'_2 & \overline{J}'_2 & J'_2 \end{bmatrix}.$$

After the LS decoupling, the spin-orbital part $P_{14}^{\sigma r}$ can be split into separate matrix elements following just the isospin separation

$$\langle P_{14}^{\sigma r}\rangle = \langle P_{14}^{\sigma}\rangle \langle P_{14}^{r}\rangle . \tag{2.27}$$

2.2.4 P_{14} action on the orbital angular momentum

For the calculation of the orbital P_{14}^r operator the basis vector must be recoupled using the recoupling coefficient with zero in the middle. This coefficient is expressed using the 6j symbol

$$\left[\begin{array}{ccc} l_{12} & \overline{L}_{12} & L_{12} \\ l_r & 0 & l_r \\ L_{12r} & \overline{L}_{12} & L \end{array}\right] \tag{2.28}$$

$$= (-1)^{l_{12r}+\overline{L}_{12}+l_r+L_{12}} \sqrt{d_{l_{12r}} d_{\overline{L}_{12}} d_{L_{12}} d_{l_r}} \left\{\begin{array}{ccc} l_{12} & \overline{L}_{12} & L_{12} \\ l_r & 0 & l_r \\ l_{12r} & \overline{L}_{12} & L \end{array}\right\}$$

$$= (-1)^{l_{12r}+\overline{L}_{12}+l_r+L_{12}} \sqrt{d_{l_{12r}} d_{L_{12}}} \left\{\begin{array}{ccc} \overline{L}_{12} & l_{12} & L_{12} \\ l_r & L & l_{12r} \end{array}\right\}.$$

By having the orbital part of the basis vector separated from the spin part, one has to recouple once again to get the form of the basis vector, where the operator P^r_{14} acts upon the desired coordinates. We need to use an additional four RECs to recouple and return to the first-hand basis vector. For the P^r_{14} operator to be applied onto state vectors we need to get the basis vector in the form

$$\left|((l_1, l_2)l_{12}, l_r)l_{12r,}(\overline{L}_1, \overline{L}_2)\overline{L}_{12})L\right\rangle. \tag{2.29}$$

This is done with help of two additional RECs

$$\left\langle((l_1, \overline{L})L_1, (l_2, \overline{L}_2)L_2)L_{12}, l_r)L \left|P^r_{14}\right| ((l'_1, \overline{L})L'_1, (l'_2, \overline{L}_2)L'_2)L'_{12}, l'_r)L\right\rangle \times\delta_{\overline{L}_1\overline{L}_2,\overline{L}'_1\overline{L}'_2} \tag{2.30}$$

$$= \left|(((l_1, \overline{L})L_1, (l_2, \overline{L}_2)L_2)L_{12}, l_r)L\right\rangle$$

$$= \sum_{l_{12}\overline{L}_{12}} \left|((l_1, l_2)l_{12}, (\overline{L}_1, \overline{L}_2)\overline{L}_{12})L_{12}, l_r)L\right\rangle \times \left[\begin{array}{ccc} l_1 & \overline{L}_1 & L_1 \\ l_2 & \overline{L}_2 & L_2 \\ l_{12} & \overline{L}_{12} & L_{12} \end{array}\right]$$

$$= \sum_{\substack{l_{12}\overline{L}_{12} \\ l_{12r}}} \left|((l_1, l_2)l_{12}, l_r)l_{12r,}(\overline{L}_1, \overline{L}_2)\overline{L}_{12})L\right\rangle \left[\begin{array}{ccc} l_{12} & \overline{L}_{12} & L_{12} \\ l_r & 0 & l_r \\ l_{12r} & \overline{L}_{12} & L \end{array}\right] \times \left[\begin{array}{ccc} l_1 & l_2 & l_{12} \\ \overline{L}_1 & \overline{L}_2 & \overline{L}_{12} \\ L_1 & L_2 & L_{12} \end{array}\right].$$

After this procedure, the action of the operator P^r_{14} consists of the modified 4HOB coefficient denoted as $\langle spec.4HOB\rangle$

$$\left\langle((l_1,\overline{L})L_1,(l_2,\overline{L}_2)L_2)L_{12},l_r)L\,|P^r_{14}|\,((l'_1,\overline{L})L'_1,(l'_2,\overline{L}_2)L'_2)L'_{12},l'_r)L\right\rangle \tag{2.31}$$

$$\times\delta_{\overline{L}_1\overline{L}_2,\overline{L}'_1\overline{L}'_2}\delta_{l_{12r},l'_{12r}}\delta_{\overline{L}_{12},\overline{L}'_{12}}$$

$$=\sum_{\substack{l_{12}\overline{L}_{12}\\ l_{12r}}}\sum_{l'_{12}}\begin{bmatrix} l_1 & \overline{L}_1 & L_1\\ l_2 & \overline{L}_2 & L_2\\ l_{12} & \overline{L}_{12} & L_{12}\end{bmatrix}\begin{bmatrix} l_{12} & l_r & l_{12r}\\ \overline{L}_{12} & 0 & \overline{L}_{12}\\ L_{12} & l_r & L\end{bmatrix}\langle spec.4HOB\rangle$$

$$\times\begin{bmatrix} l'_{12} & \overline{L}_{12} & L'_{12}\\ l'_r & 0 & l'_r\\ l_{12r} & \overline{L}_{12} & L\end{bmatrix}\begin{bmatrix} l'_1 & l'_2 & l'_{12}\\ \overline{L}_1 & \overline{L}_2 & \overline{L}_{12}\\ L'_1 & L'_2 & L'_{12}\end{bmatrix}.$$

The 4HOB coefficient matrix element is denoted as

$$\left\langle(e_1l_1,e_2l_2)\,l_{12},e_rl_r:l_{12r}|\,(e'_1l'_1,e'_2l'_2)\,l'_{12},e'_rl'_r:l'_{12r\ d_1d_2}\right\rangle\delta_{l_{12r},l_{12r}}. \tag{2.32}$$

For the correct representation of the P_{14} in the HO basis, one has to determine correct values for the mass-ratio parameters [62]. This is done in the Jacobi coordinate representation. The standard 4HOB notation [63] for the transformation factorization is

$$\begin{pmatrix}\rho_1\\ \rho_2\\ \rho_3\end{pmatrix}=\begin{pmatrix}\sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0\\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}1 & 0 & 0\\ 0 & \sqrt{\frac{d_2}{1+d_2}} & \sqrt{\frac{1}{1+d_2}}\\ 0 & \sqrt{\frac{1}{1+d_2}} & -\sqrt{\frac{d_2}{1+d_2}}\end{pmatrix} \tag{2.33}$$

$$\times\begin{pmatrix}\sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0\\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}\rho'_1\\ \rho'_2\\ \rho'_3\end{pmatrix}$$

The Jacobi coordinates which are affected by the operator action are presented in eq.(2.8). The orthogonal transformation matrix from particle to Jacobi coordinates is written as:

$$\begin{pmatrix} \rho_1^1 \\ \rho_2^1 \\ \rho_1^2 \\ \rho_2^2 \\ \rho_r \\ \rho_0 \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} & 0 & 0 & 0 \\ 0 & \sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} \\ 0 & 0 & 0 & 0 & \sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{2}} \\ \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} \\ \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} \end{pmatrix} \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \\ r_6 \end{pmatrix}. \tag{2.34}$$

In the one particle coordinate basis, the operator $\langle r \left| P_{14}^r \right| r' \rangle$ is equal to

$$\langle r' | P_{14} | r \rangle = \begin{pmatrix} r'_1 \\ r'_2 \\ r'_3 \\ r'_4 \\ r'_5 \\ r'_6 \end{pmatrix} \cdot \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \\ r_6 \end{pmatrix}. \tag{2.35}$$

By using the orthogonal transformation from eq.(2.34) and the operator representation in the one particle coordinate basis in eq.(2.35), the representation of P_{14} in the Jacobi coordinates is found to be equal to

$$\begin{pmatrix} \rho_1^{1'} \\ \rho_2^{1'} \\ \rho_1^{2'} \\ \rho_2^{2'} \\ \rho_1' \\ \rho_0' \end{pmatrix} \begin{pmatrix} \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} & 0 & 0 & 0 \\ 0 & \sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} \\ 0 & 0 & 0 & 0 & \sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{2}} \\ \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} \\ \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} \end{pmatrix}$$

$$\times \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{2.36}$$

$$\times \begin{pmatrix} \frac{1}{3}\sqrt{2}\sqrt{3} & 0 & 0 & 0 & \frac{1}{6}\sqrt{6} & \frac{1}{6}\sqrt{6} \\ -\frac{1}{6}\sqrt{6} & \frac{1}{2}\sqrt{2} & 0 & 0 & \frac{1}{6}\sqrt{6} & \frac{1}{6}\sqrt{6} \\ -\frac{1}{6}\sqrt{6} & -\frac{1}{2}\sqrt{2} & 0 & 0 & \frac{1}{6}\sqrt{6} & \frac{1}{6}\sqrt{6} \\ 0 & 0 & \frac{1}{3}\sqrt{2}\sqrt{3} & 0 & -\frac{1}{6}\sqrt{6} & \frac{1}{6}\sqrt{6} \\ 0 & 0 & -\frac{1}{6}\sqrt{6} & \frac{1}{2}\sqrt{2} & -\frac{1}{6}\sqrt{6} & \frac{1}{6}\sqrt{6} \\ 0 & 0 & -\frac{1}{6}\sqrt{6} & -\frac{1}{2}\sqrt{2} & -\frac{1}{6}\sqrt{6} & \frac{1}{6}\sqrt{6} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{3} & 0 & \frac{2}{3} & 0 & -\frac{2}{3} & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ \frac{2}{3} & 0 & \frac{1}{3} & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -\frac{2}{3} & 0 & \frac{2}{3} & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \rho_1^1 \\ \rho_2^1 \\ \rho_1^2 \\ \rho_2^2 \\ \rho_1 \\ \rho_0 \end{pmatrix}.$$

The relevant part of the representation is the 3×3 matrix, which acts upon coordinates of first and fourth quasiparticle

$$\begin{pmatrix} \rho_1^{1'} \\ \rho_1^{2'} \\ \rho_r' \end{pmatrix} = \begin{pmatrix} \frac{1}{3} & \frac{2}{3} & -\frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} & \frac{2}{3} \\ -\frac{2}{3} & \frac{2}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} \rho_1^1 \\ \rho_1^2 \\ \rho_r \end{pmatrix}. \tag{2.37}$$

Then the mass-ratio parameters of the Standard Talmi-Moshinsky transformations are calculated algebraically:

$$\begin{pmatrix} a & A & 0 \\ A & -a & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & b & B \\ 0 & B & -b \end{pmatrix} \begin{pmatrix} a & A & 0 \\ A & -a & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} bA^2 + a^2 & -Aa\,(b-1) & AB \\ -Aa\,(b-1) & A^2 + ba^2 & -Ba \\ AB & -Ba & -b \end{pmatrix}. \tag{2.38}$$

The mass-ratio parameter d_2 :

$$-b = \frac{1}{3}; b = -\frac{1}{3} = -\sqrt{\frac{d_2}{1+d_2}}; \frac{1}{3} = \sqrt{\frac{d_2}{1+d_2}}; d_2 = \frac{1}{8}. \tag{2.39}$$

The mass-ratio parameter d_1 :

$$AB = \frac{2}{3}; \sqrt{\frac{1}{1+d_1}}\sqrt{\frac{1}{1+d_2}} = \frac{2}{3}; \sqrt{\frac{1}{1+d_1}}\sqrt{\frac{1}{1+\frac{1}{8}}} = \frac{2}{3}; d_1 = 1. \tag{2.40}$$

By putting calculated d parameters in the 4HOB Jacobi coordinate representation we get the correct values though the minus signs are off

$$\begin{pmatrix} \sqrt{\frac{1}{1+1}} & \sqrt{\frac{1}{1+1}} & 0 \\ \sqrt{\frac{1}{1+1}} & -\sqrt{\frac{1}{1+1}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{\frac{\frac{1}{8}}{1+\frac{1}{8}}} & \sqrt{\frac{1}{1+\frac{1}{8}}} \\ 0 & \sqrt{\frac{1}{1+\frac{1}{8}}} & -\sqrt{\frac{\frac{1}{8}}{1+\frac{1}{8}}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{1}{1+1}} & \sqrt{\frac{1}{1+1}} & 0 \\ \sqrt{\frac{1}{1+1}} & -\sqrt{\frac{1}{1+1}} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{2}{3} & \frac{1}{3} & \frac{2}{3} \\ \frac{1}{3} & \frac{2}{3} & -\frac{2}{3} \\ \frac{2}{3} & -\frac{2}{3} & -\frac{1}{3} \end{pmatrix}. \tag{2.41}$$

The expression is not equal to the P_{14} coordinate representation to the full extent. The two additional phasis multipliers $(-1)^{l_r}$ and $(-1)^{\lambda_2'}$ are needed for the appropriate orientation of the coordinate vectors ρ_r and ρ_1^2. Then we get the correct representation

$$\begin{pmatrix} \sqrt{\frac{1}{1+1}} & \sqrt{\frac{1}{1+1}} & 0 \\ \sqrt{\frac{1}{1+1}} & -\sqrt{\frac{1}{1+1}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{\frac{\frac{1}{8}}{1+\frac{1}{8}}} & \sqrt{\frac{1}{1+\frac{1}{8}}} \\ 0 & \sqrt{\frac{1}{1+\frac{1}{8}}} & -\sqrt{\frac{\frac{1}{8}}{1+\frac{1}{8}}} \end{pmatrix} \tag{2.42}$$

$$\times \begin{pmatrix} \sqrt{\frac{1}{1+1}} & \sqrt{\frac{1}{1+1}} & 0 \\ \sqrt{\frac{1}{1+1}} & -\sqrt{\frac{1}{1+1}} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{3} & \frac{2}{3} & -\frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} & \frac{2}{3} \\ -\frac{2}{3} & \frac{2}{3} & \frac{1}{3} \end{pmatrix}.$$

The final expression of $\langle P_{14} \rangle$ matrix element consists of the products of the matrix elements composing the expressions from eq.(2.24), eq.(2.26) and eq.(2.31).

In this section, the approach of the calculation of the CFPs using the Λ operator formalism in the Jacobi coordinates is presented. It was shown that in the coupled-J scheme the calculations depend heavily on the angular momenta algebra, and can become complicated. This can be made easier if one has methodical approach for derivation. One of the key features is the square bracket notation of the RECs. The CFPs for the six body system are acquired by the direct diagonalization of the calculated P_{14} matrix. The eigenvectors corresponding to the antisymmetric subspace $[1^6]$ are the CFPs.

2.3 Computation of the CFPs

In this section, we present an approach for the computation of the CFPs for the six nucleon system. An algorithm must be carefully thought through as the computation time and the accuracy depends on the approach. Firstly, we need to construct the CFPs of the three-particle subclusters of the six nucleon system. We start from the binary cluster basis vector

$$\langle((E_1 J_1 T_1, E_2 J_2 T_2)\bar{J}T, e_r l_r) E_6 JT \mid . \tag{2.43}$$

representation. Here $E_1 J_1 T_1$ is the quantum numbers of the first cluster and $E_2 J_2 T_2$ quantum numbers of the second cluster. Their

total angular momenta J_1 and J_2 are coupled resulting in the intermediate momenta $\bar{J}$. $\bar{J}$ is then coupled with the quantum number l_r, representing the relative motion of the two subclusters. Coupling results in the total angular momentum J. This basis vector has an internal structure. As each of the subclusters is divided as the $1+2$ system, we have the quantum numbers $(\epsilon_1\lambda_1 s_1)j_1$ representing the first nucleon and quantum numbers $(\bar{E}_1\bar{L}_1\bar{S}_1)J_1$ representing the second and third nucleons of the first cluster. In the first ensemble ϵ_1 is the HO energy, λ_1 is the momentum, s_1 is the spin and j_1 is the total angular momentum. In the second ensemble $\bar{E}_1$ is the HO energy, $\bar{L}_1$ is the angular momentum, $\bar{S}_1$ is the spin and J_1 is the total angular momentum. The structure of the basis vector for the second cluster is the same.

We need to calculate the permutation elements P_{13} and P_{46} of the symmetric group S_3 in the binary cluster representation. The calculation of P_{46} is the same as the calculation of P_{13} . The only difference is the basis vector states on which the permutation elements act upon. For P_{13} we have

$$\begin{aligned}&\langle[(\epsilon_1\lambda_1 s_1)j_1,(\bar{E}_1\bar{L}_1\bar{S}_1)J_1;(\tau_1,\bar{T}_1)T_1]\mid P_{13}\mid\\&\times[(\epsilon_1'\lambda_1' s_1')j_1',(\bar{E}_1'\bar{L}_1'\bar{S}_1')J_1';(\tau_1',\bar{T}_1')T_1']\rangle^{E_1J_1T_1}\end{aligned}\tag{2.44}$$

and for P_{46}

$$\begin{aligned}&\langle[(\epsilon_2\lambda_2 s_2)j_2,(\bar{E}\bar{L}_2\bar{S}_2)J_2;(\tau_2,\bar{T}_2)T_2]\mid P_{46}\mid\\&\times[(\epsilon_2'\lambda_2' s_2')j_2',(\bar{E}_2'\bar{L}_2'\bar{S}_2')J_2';(\tau_2',\bar{T}_2')T'_2]\rangle^{E_2J_2T_2}.\end{aligned}\tag{2.45}$$

The permutation elements are calculated after ensuring the antisymmetric subspace $[1^2]$ for the two particle Jacobi coordinates for each cluster. This operation is done relatively easy, as the symmetric group S_2 has only two irreducible representations: the antisymmetric $[1^2]$ and the symmetric $[2]$. This restriction on the subspace can be ensured by the condition $(-1)^\mu = \pm 1$. μ is the set of quantum numbers representing the subspaces, where symmetric $(+1)$ or antisymmetric(-1) irreps must be distinguished. When the antisymmetric two nucleon subspace is ensured, the only subspaces for the three-nucleon system can be $[1^3][1^2]$ and $[21][1^2]$. To find

the subspaces we need to diagonalize the matrices of the operators. The CFPs for the subclusters are determined by the eigenvalues of the diagonalized matrix. They correspond to the irreps. The eigenvalues are determined by the eq.(1.36). We characterize the CFPs for three-particle subclusters with bra-kets

$$\langle[(\epsilon_1\lambda_1 s_1)j_1,(\bar{E}_1\bar{L}_1\bar{S}_1)J_1;(\tau_1,\bar{T}_1)T_1]\mid E_1J_1T_1[1^3]\gamma_1\rangle \tag{2.46}$$

and

$$\langle[(\epsilon_2\lambda_2 s_2)j_2,(\bar{E}_2\bar{L}_2\bar{S}_2)J_2;(\tau_2,\bar{T}_2)T_2]\mid E_2J_2T_2[1^3]\gamma_2\rangle. \tag{2.47}$$

In these bra-kets the quantum number γ_x is the additional quantum number which characterizes the repetition of the irrep $[1^3]$. Subscript x denotes the number of the subcluster.

For each calculated matrix we have the two dimensions: the dimension of undiagonalized matrix with a restricted subspace $[1^2]$ - $b\dim_x$ and the dimensions of the projection to the irreducible representation $[1^3][1^2]$ - $f\dim_x$. We construct the CFPs for the six body system by the superposition of the CFPs of three-particle subclusters. The group chain for this procedure is $S_6 \supset S_3 \times S_3$. To get the six body CFPs we must calculate the inter-cluster transposition operator P_{14} of the symmetric group S_6 in the basis of the superposition of three particle CFPs. The operator P_{14} is calculated without any assumption of the aforementioned symmetry of $[1^3][1^2]$:

$$\begin{gathered}\langle(\{[(\epsilon_1\lambda_1 s_1)j_1,(\bar{E}_1\bar{L}_1\bar{S}_1)J_1;(\tau_1,\bar{T}_1)T_1]\times \\ [(\epsilon_2\lambda_2 s_2)j_2,(\bar{E}_2\bar{L}_2\bar{S}_2)J_2;(\tau_2,\bar{T}_2)T_2]\}\bar{J},l_r)JT\mid .\end{gathered} \tag{2.48}$$

Then the calculated matrix is transformed into the basis vector where the symmetry is ensured according to the aforementioned group chain

$$\begin{gathered}\langle(\{[(\epsilon_1\lambda_1 s_1)j_1,(\bar{E}_1\bar{L}_1\bar{S}_1)J_1;(\tau_1,\bar{T}_1)T_1]\times \\ [(\epsilon_2\lambda_2 s_2)j_2,(\bar{E}_2\bar{L}_2\bar{S}_2)J_2;(\tau_2,\bar{T}_2)T_2]\}\bar{J},l_r)JT\mid \times \\ \{E_1J_1T_1[1^3]\gamma_1\}\otimes\{E_2J_2T_2[1^3]\gamma_2\}\rangle.\end{gathered} \tag{2.49}$$

To do this procedure we start by ensuring the antisymetric two particle subspace of the six particle system. Then following the group chain $S_3 \supset S_2$ we ensure the antisymmetric subspace $[1^3][1^2]$ for three-particle subsystem. Then for the full six particle system we get four possible irrep configurations- $[1^6][1^3][1^3]$, $[21^4][1^3][1^3]$, $[2^21^2][1^3][1^3]$, $[2^3][1^3][1^3]$. For the antisymmetric states we only need the irrep labelled as $[1^6]$. The dimension of the matrix of P_{14} in the antisymmetric three-particle subsystems space is equal to the product of the dimensions of the antisymmetric subcluster states. The computational scheme for the calculation is presented in fig.(2.4). The bra-ket representing the transformation of the first cluster is

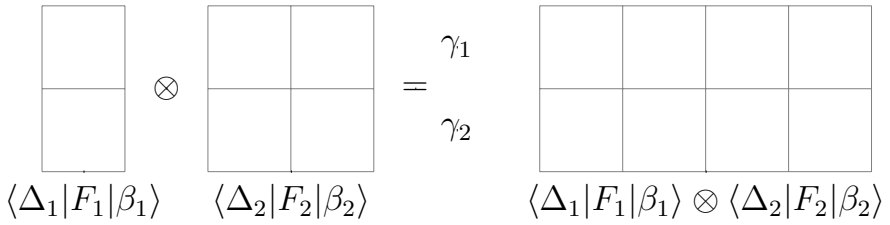


Figure 2.4: Scheme for computation of the CFPs for the subclusters. We calculate the superposion of the transformations from state vectors without any antisymmetry to antisymmetric with respect to the subclusters. β_x is ket without any consideration of the antisymmetry, Δ_x is bra denoting antisymmetric three-particle subcluster states, x is the number of the subcluster, γ_x is the number of the repetition of the antisymmetric irrep $[1^3]$.

denoted as $\langle\Delta_1|F_1|\beta_1\rangle$. Where

$$|\beta_1\rangle = |(\epsilon_1\lambda_1 s_1)j_1, (\bar{E}_1\bar{L}_1\bar{S}_1)J_1; (\tau_1, \bar{T}_1)T_1\rangle \tag{2.50}$$

is the HO ket without any consideration for the symmetry and

$$\langle\Delta_1| = \langle E_1 J_1 T_1 [1^3]\gamma_1| \tag{2.51a}$$

is bra denoting antisymmetric three-particle subcluster states. For the second cluster, we have analogical bra-ket $\langle\Delta_2|F_2|\beta_2\rangle$. P_{14} is calculated in the basis

$$\langle(\beta_1 \otimes \beta_2)|P_{14}|(\beta_1 \otimes \beta_2)\rangle^{E_1 J_1 T_1; E_2 J_2 T_2}. \tag{2.52}$$

Then it is transformed into the basis vector

$$\langle\alpha| = \langle\{E_1 J_1 T_1 [1^3]\gamma_1\} \otimes \{E_2 J_2 T_2 [1^3]\gamma_2\}|. \tag{2.53}$$

The superscript $E_1 J_1 T_1; E_2 J_2 T_2$ denotes the matrix of the P_{14} for the particular values of the three-particle subclusters. The transformation is done by using the aforementioned eigenvectors (fig.(2.5)). The eigenvector superposition is constructed depending on the repetition of the needed irrep. This is determined by the additional quantum number γ_x. Finally, after all these steps the operator is diagonalized and the eigenvectors corresponding to the irrep $[1^6]$ are selected. This completes the construction of the transition matrix to the basis vector $|EJT[1^6]\Gamma\rangle$. E is HO quanta for the whole system, J is the total angular momentum, T is the isospin of the system and Γ is the additional quantum number, enumerating the irreps. After this procedure is finished, we arrive at the CFPs for the six body system

$$\langle\{E_1 J_1 T_1 [1^3]\gamma_1\} \otimes \{E_2 J_2 T_2 [1^3]\gamma_2\}|EJT[1^6]\Gamma\rangle. \tag{2.54}$$

For illustration purposes, the number of the three-nucleon states corresponding to each irrep of the operator P_{13}, as well as, the six nucleon states corresponding to each irrep of the operator P_{14} have been calculated. This procedure was done for different HO energy quanta, total angular momentum, and the total isospin values. One can see the evolution of the number of antisymmetrical states in the three-nucleon (tbl.(2.1)) and the six nucleon systems (tbl.(2.2)). We choose the system with quantum numbers $J = 1$ and $T = 1$ to demonstrate the antisymmetric state calculation procedure for the three-nucleon system.

When $J = 2$ and $T = 2$ (corresponds to ${}^6_1\mathrm{H}$) (tbl.(2.2)), we get no antisymmetric states at the HO energy 1 and 2, only states with lower degree of antisymmetry. First completely antisymmetrical states appear at the HO energy equal to 3. We get a total matrix dimension equal to 212 and the number of antisymmetric states is 4.

When $J = 0$ and $T = 1$ (corresponds to ${}^6_2\mathrm{He}$ and ${}^6_4\mathrm{Be}$) we get the first two fully antisymmetric states when HO energy is equal to 2. The antisymmetric states for $J = 1$, $T = 0$ (Corresponds to ${}^6_3\mathrm{Li}$)

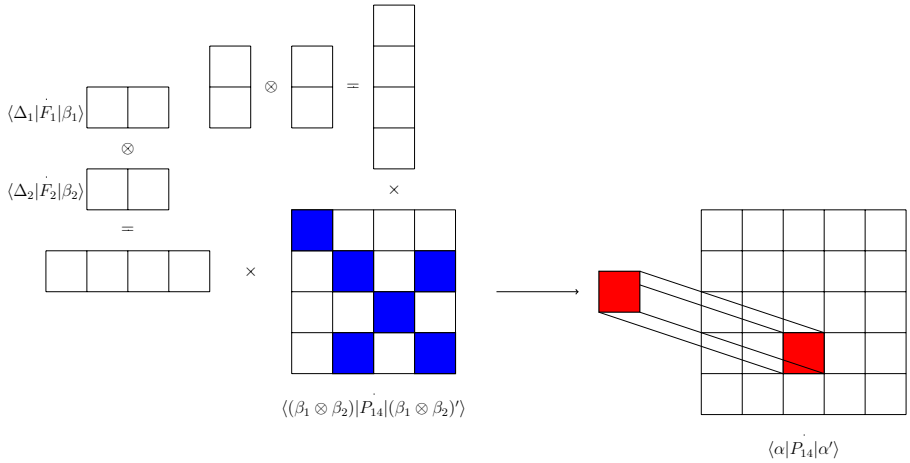


Figure 2.5: The procedure for the transformation of the P_{14} from HO basis to the antisymmetric three-particle subcluster basis. The matrix of the operator P_{14} is multiplied by the eigenvector matrices. They represent the transformation from state vectors without any antisymmetry to the antisymmetric states. β_x is ket without any consideration of the antisymmetry, Δ_x is bra denoting antisymmetric three-particle subcluster states, x is the number of the subcluster, γ_x is the number of the repetition of the antisymmetric irrep $[1^3]$, α and α' denote the superposition of the antisymmetric two three-particle subclusters.

follow the same path. We get only states with partial antisymmetry when the HO quanta is equal to 0 and 1. For this stable isotope when the HO quanta is greater than 1 the amount of the generated antisymmetrical states is bigger than for other elements. The obtained computational results confirm the predicted eigenvalues of the operators P_{13} and P_{14}.

In this section we introduced the algebraic method for CFP calculation of the six nucleon system. This formalism allows the c.m. motion states to be easily excluded in the HO basis, and at the same time the good quantum numbers are maintained. The generated basis vector spaces for different isotopes are small. This is the direct result of the application of the CFP formalism using the Jacobi coordinates in the coupled angular momentum basis vector.

Table 2.1: The calculation of the three-body antisymmetric states. The states are calculated for J=1, T=1. E is HO energy, Dim - dimension of matrix. The eigenvalue -1 corresponds to the antisymmetric state $[1^3]$. The eigenvalue -$\frac{1}{2}$ corresponds to the antisymmetric state of lesser degree [21].

E	Dim	-1	$-\frac{1}{2}$	E	Dim	-1	$-\frac{1}{2}$
0	2	1	1	16	306	102	204
1	6	2	4	17	342	114	228
2	12	4	8	18	380	127	253
3	20	7	13	19	420	140	280
4	30	10	20	20	462	154	308
5	42	14	28	21	506	169	337
6	56	19	37	22	552	184	368
7	72	24	48	23	600	200	400
8	90	30	60	24	650	217	433
9	110	37	73	25	702	234	468
10	132	44	88	26	756	252	504
11	156	52	104	27	812	271	541
12	182	61	121	28	870	290	580
13	210	70	140	29	930	310	620
14	240	80	160	30	992	331	661
15	272	91	181	31	1056	352	704

Table 2.2: Calculation of eigenvalues correspoding to the irreps for six body systems. E is HO energy quanta; J is total angular momentum; T is isospin; Dimension is size of calculated P_{14} matrix; Numbers are corresponding eigenvalues. J=0 and T=1 corresponds to $^{6}_{2}$He or $^{6}_{4}$Be ground states; J=1, T=0 corresponds to $^{3}_{3}$Li; J=2,T=2 correspond to $^{5}_{1}$H. Calculations were performed with supercomputer "HPC Sauletekis" [64], using 3 nodes (36 cores). We used standard Double precision for calculation of the matrix and library "ScaLAPACK" for parallelism of the calculation.

E	J	T	*Dimension*	-1	$-\frac{1}{3}$	$\frac{1}{9}$	$\frac{1}{3}$
0	1	0	1	0	0	1	0
1	1	0	10	0	2	5	3
2	1	0	63	3	12	33	15
3	1	0	282	11	63	132	76
4	1	0	1007	45	231	476	255
5	1	0	2035	86	472	947	530
6	1	0	8285	387	1988	3807	2103
1	2	2	2	0	0	1	1
2	2	2	33	0	5	16	12
3	2	2	212	4	40	101	67
4	2	2	925	24	193	436	272
5	2	2	3202	103	704	1493	902
6	2	2	9457	346	2150	4373	2588
0	0	1	1	0	0	1	0
1	0	1	7	0	1	4	2
2	0	1	44	2	8	24	10
3	0	1	192	7	41	93	51
4	0	1	679	29	151	326	173
5	0	1	2035	86	472	947	530
6	0	1	5434	244	1281	2518	1391

Chapter 3

Higher-order Talmi-Moshinsky transformations

In the previous chapter, we used an algebraic approach to construct the antisymmetric state vectors of the six nucleon system. While the spin and the isospin parts of the operator P_{14} were calculated relatively easy, the orbital part needed special care. To calculate the orbital part we had to use the Talmi-Moshinsky transformation and corresponding brackets. Special construction of three harmonic oscillator brackets and RECs was used to tackle this problem. The number of transformed Jacobi coordinates depends on the partition of the system (corresponds to the particular Jacobi tree) and the initial antisymmetrization of the N particle system. So it would be useful to have these constructions of multiple Talmi-Moshinsky transformations generalized and formulated as tools for the calculation of transposition operators of the symmetric group.

3.1 Brackets for three Jacobi coordinates

In this section, we present the transformation brackets for three Jacobi coordinates (4HOB). Three Jacobi coordinates are involved in the coordinate transformation if no less than four particles are affected by the transformation. These coefficients are used for the representation of a higher-order Talmi-Moshinsky transformation

in the HO basis. 4HOBs are studied extensively in [60, 62, 63, 65]. 4HOBs are defined as the three-dimensional coordinate transformation parameterized by three Euler angles α, β, γ. A case when $\alpha = \gamma$ is the most interesting for the transposition operator calculation. In this case, the three-dimensional transformation, acting upon the Jacobi coordinates $\begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{pmatrix}$ can be written as a product of three matrices. These matrices represent the two-dimensional transformations and implement the group chain $SO_3 \supset SO_2$. In matrix form it can be written as

$$\begin{pmatrix} \rho_1' \\ \rho_2' \\ \rho_3' \end{pmatrix} \begin{pmatrix} \sin(\alpha) & \cos(\alpha) & 0 \\ \cos(\alpha) & -\sin(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sin(\beta) & \cos(\beta) \\ 0 & \cos(\beta) & -\sin(\beta) \end{pmatrix} \times \begin{pmatrix} \sin(\alpha) & \cos(\alpha) & 0 \\ \cos(\alpha) & -\sin(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{pmatrix}. \tag{3.1}$$

The direct calculation of this transformation is complicated and a more handy approach is the calculation of three two-dimensional transformations. The Talmi-Moshinsky coordinate transformation is defined as the two-dimensional matrix $\begin{pmatrix} \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} \\ \sqrt{\frac{1}{1+d}} & -\sqrt{\frac{d}{1+d}} \end{pmatrix}$. It is used to express the four-particle Talmi-Moshinsky transformation as the product of these standard transformations. The four-particle Talmi-Moshinsky transformation depends on the parameters d_1, d_2. They correspond to Euler angles as

$$T_{12}(d_1)T_{23}(d_2)T_{12}(d_1) = \tag{3.2}$$
$$\begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{\frac{d_2}{1+d_2}} & \sqrt{\frac{1}{1+d_2}} \\ 0 & \sqrt{\frac{1}{1+d_2}} & -\sqrt{\frac{d_2}{1+d_2}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The aforementioned coordinate transformation is represented in the HO basis. It results in the three two dimensional HOBs and summation over the intermediate states. Since we are working in the

coupled angular momenta basis, this operation involves RECs. The definition of the four-particle wavefunction in intrinsic (Jacobi) coordinates $\boldsymbol{\rho_n}$ with coupled momenta is

$$\begin{aligned}&\{\{\phi_{e_1l_1}(\boldsymbol{\rho}_1)\otimes\phi_{e_2l_2}(\boldsymbol{\rho}_2)\}_{L_{12}}\otimes\phi_{e_3l_3}(\boldsymbol{\rho}_3)\}_{LM}= \\ &\sum_{m_1m_2M_{12}m_3} C^{L_{12}M_{12}}_{l_1m_1l_2m_2}C^{LM}_{L_{12}M_{12}l_3m_3}\phi_{e_1l_1m_1}(\boldsymbol{\rho}_1) \\ &\times\phi_{e_2l_2m_2}(\boldsymbol{\rho}_2)\phi_{e_3l_3m_3}(\boldsymbol{\rho}_3).\end{aligned} \tag{3.3}$$

$\phi_{e_xl_xm_x}(\boldsymbol{\rho}_x)$ is the HO function defined as

$$\phi_{elm}(\boldsymbol{\rho}) = (-1)^n\left[\frac{2\,(n!)}{\Gamma\,(n+l+3/2)}\right]^{\frac{1}{2}} e^{\left(-\rho^2/2\right)}\rho^l L_n^{(l+1/2)}\left(\rho^2\right)Y_{lm}\left(\boldsymbol{\rho}/\rho\right). \tag{3.4}$$

Let us write a state vector for such transformation using bra-ket notation as

$$\langle((e_1l_1,e_2l_2)l_{12},e_3l_3)l|. \tag{3.5}$$

The variables e_xl_x correspond to the HO energy quanta and the angular momentum in line with the Jacobi coordinate ρ_x (For example, the coordinate ρ_1 will correspond to quantum numbers e_1l_1.). To get the representation of eq.(3.2) in the HO basis we need to know how to calculate then matrix element in the basis vector from eq.(3.5)

$$\langle((e_1l_1,e_2l_2)l_{12},e_3l_3)l|T_{12}(d_1)T_{23}(d_2)T_{12}(d_1)|((e_1'l_1',e_2'l_2')l_{12}',e_3'l_3')l\rangle. \tag{3.6}$$

A practical way to calculate this matrix element is to split it for each transformation, to calculate them separately, and then to assemble the results. The transformation $T_{12}(d_1)$ acting on the basis vector $\langle((e_1l_1,e_2l_2)l_{12},e_3l_3)l|$ does not require any additional action. It results in Dirac delta function for the quantum numbers which are not affected by the transformation:

$$\begin{aligned}&\langle((e_1l_1,e_2l_2)l_{12},e_3l_3)l|T_{12}(d_1)|((e_1'l_1',e_2'l_2')l_{12}',e_3'l_3')l\rangle= \\ &\quad\langle((e_1l_1,e_2l_2)l_{12}|T_{12}(d_1)|((e_1'l_1',e_2'l_2')l_{12}'\rangle\delta_{l_{12}e_3l_3l,l_{12}'e_3'l_3'l'}.\end{aligned} \tag{3.7}$$

The next transformation to be applied is $T_{23}(d_2)$. The basis vector has to be recoupled in a way that it becomes suitable for the application of this transformation. It has to act upon the correct quantum numbers, so the basis vector $\langle((e_1l_1, e_2l_2)l_{12}, e_3l_3)l|$ must be transformed to assume the form $\langle((e_1l_1, (e_2l_2, e_3l_3)l_{23})l|$. Such transformations are performed using RECs. In the bra-ket notation, they are denoted

$$\langle((l_1, l_2)L_{12}, (l_3, l_4)L_{34})L|((l_1, l_3)L_{13}, (l_2, l_4)L_{24})L\rangle\,. \tag{3.8}$$

We rewrite them using the square bracket notation as

$$\langle((l_1, l_2)L_{12}, (l_3, l_4)L_{34})L|((l_1, l_3)L_{13}, (l_2, l_4)L_{24})L\rangle = \begin{bmatrix} l_1 & l_3 & L_{13} \\ l_2 & l_4 & L_{24} \\ L_{12} & L_{34} & L \end{bmatrix}. \tag{3.9}$$

To recouple the basis vector $\langle((e_1l_1, e_2l_2)l_{12}, e_3l_3)l|$ to apply the transformation $T_{23}(d_2)$ we use the recoupling coefficient with one zero value

$$\langle((e_1l_1, e_2l_2)l_{12}, e_3l_3)l|((e_1l_1, (e_2l_2, e_3l_3)l_{23})l\rangle = \begin{bmatrix} l_1 & 0 & l_1 \\ l_2 & l_3 & L_{23} \\ L_{12} & l_3 & L \end{bmatrix} \tag{3.10}$$

Since the 9j symbol contain zero, the expression in eq.(1.69) will result in a REC with 6j symbol following the eq.(1.73)

$$\begin{bmatrix} l_1 & 0 & l_1 \\ l_2 & l_3 & L_{23} \\ L_{12} & l_3 & L \end{bmatrix} = (-1)^{l_2+L+l_3+l_1}\sqrt{d_{L_{12}}d_{L_{23}}} \begin{Bmatrix} l_1 & l_2 & L_{12} \\ l_3 & L & L_{23} \end{Bmatrix}.$$

For the reversed REC $\langle((e_1l_1, (e_2l_2, e_3l_3)l_{23})l|((e_1l_1, e_2l_2)l_{12}, e_3l_3)l\rangle$ the same approach is followed relying on the eq.(1.73). This coefficient results in a matrix with a zero on the left part of square bracket

$$\begin{bmatrix} l_1 & l_2 & L_{12} \\ 0 & l_3 & l_3 \\ l_1 & L_{23} & L \end{bmatrix} = (-1)^{l_2+L+l_3+l_1}\sqrt{d_{L_{23}}d_{L_{12}}} \begin{Bmatrix} l_3 & l_2 & L_{23} \\ l_1 & L & L_{12} \end{Bmatrix}. \tag{3.11}$$

Now when we know how to calculate the recoupling coefficients we can write the full expression for a matrix element in eq.(3.6). The expression will include seven sums over the intermediate variables, required for intermediate basis vector. These sums run over three individual transformations T_{12}, T_{23}, T_{12} and the recoupling coefficients

$$\langle((e_1l_1,e_2l_2)l_{12},e_3l_3)l|T_{12}(d_1)T_{23}(d_2)T_{12}(d_1)|((e'_1l'_1,e'_2l'_2)l'_{12},e'_3l'_3)l\rangle_{d_1d_2} = \tag{3.12}$$

$$\sum_{\substack{\varepsilon_1\lambda_1,\varepsilon_2\lambda_2,\Lambda_{23}\\ \varepsilon'_2\lambda'_2}} \langle((e_1l_1,e_2l_2)L_{12},e_3l_3)L|T_{12}(d_1)|((\varepsilon_1\lambda_1,\varepsilon_2\lambda_2)L_{12},e_3l_3)L\rangle$$

$$\times \begin{bmatrix} \lambda_1 & 0 & \lambda_1 \\ \lambda_2 & l_3 & \Lambda_{23} \\ L_{12} & l_3 & L \end{bmatrix}$$

$$\times \langle(\varepsilon_1\lambda_1,(\varepsilon_2\lambda_2,e_3l_3)\Lambda_{23})L|\,T_{23}(d_2)|(\varepsilon_1\lambda_1,(\varepsilon'_2\lambda'_2,e'_3l'_3)\Lambda_{23})L\rangle$$

$$\times \begin{bmatrix} \lambda_1 & \lambda'_2 & L'_{12} \\ 0 & l'_3 & l'_3 \\ \lambda_1 & \Lambda_{23} & L \end{bmatrix}$$

$$\times\langle((\varepsilon_1\lambda_1,\varepsilon'_2\lambda'_2)L'_{12},e'_3l'_3)L|T_{12}(d_1)|((e'_1l'_1,e'_2l'_2)L'_{12},e'_3l'_3)L\rangle.$$

For quantum numbers unaffected by the two particle transformations the Dirac delta functions are introduced. Taking them into account we arrive at the expression

$$\langle((e_1l_1,e_2l_2)l_{12},e_3l_3)l|T_{12}(d_1)T_{23}(d_2)T_{12}(d_1)|((e'_1l'_1,e'_2l'_2)l'_{12},e'_3l'_3)l\rangle_{d_1d_2} = \tag{3.13}$$

$$\sum_{\substack{\varepsilon_1\lambda_1,\varepsilon_2\lambda_2,\Lambda_{23}\\ \varepsilon'_2\lambda'_2}} \langle e_1l_1,e_2l_2:L_{12}|\varepsilon_1\lambda_1,\varepsilon_2\lambda_2:L_{12}\rangle_{d_1}\delta_{L_{12}e_3l_3,L'_{12}e'_3l'_3}$$

$$\times \begin{bmatrix} \lambda_1 & 0 & \lambda_1 \\ \lambda_2 & l_3 & \Lambda_{23} \\ L_{12} & l_3 & L \end{bmatrix} \langle\varepsilon_2\lambda_2,e_3l_3:\Lambda_{23}|\varepsilon'_2\lambda'_2,e'_3l'_3:\Lambda_{23}\rangle_{d_2}$$

$$\times \begin{bmatrix} \lambda_1 & \lambda'_2 & L'_{12} \\ 0 & l'_3 & l'_3 \\ \lambda_1 & \Lambda_{23} & L \end{bmatrix} \langle\varepsilon_1\lambda_1,\varepsilon'_2\lambda'_2:L_{12}|e'_1l'_1,e'_2l'_2:L'_{12}\rangle_{d_1}\delta_{L_{12},L'_{12}}.$$

The two particle transformations results in two particle HOBs. We now have constructed higher-order Talmi-Moshinsky brackets for the calculation of the permutation operators in the HO basis. This construction is called the four particle harmonic oscillator brackets or 4HOB. This "building block" is useful when the three Jacobi coordinates are involved in calculation of the permutation operator.

3.1.1 Factorization of 4HOBs

In this section, we present the method for the factorization of the 4HOB transformation using methods described in [62]. The 4HOB transformation is symmetric in respect to the central transformation $T_{23}(d_2)$ and can be factorized as

$$T_{23}(d_2) = T_{23}(x) F T_{23}(x). \tag{3.14}$$

In the Jacobi coordinate basis, the factorization of the $T_{23}(d_2)$ can be written as

$$\begin{pmatrix} \sqrt{\frac{d_2}{1+d_2}} & \sqrt{\frac{1}{1+d_2}} \\ \sqrt{\frac{1}{1+d_2}} & -\sqrt{\frac{d_2}{1+d_2}} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{x}{1+x}} & \sqrt{\frac{1}{1+x}} \\ \sqrt{\frac{1}{1+x}} & -\sqrt{\frac{x}{1+x}} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \sqrt{\frac{x}{1+x}} & \sqrt{\frac{1}{1+x}} \\ \sqrt{\frac{1}{1+x}} & -\sqrt{\frac{x}{1+x}} \end{pmatrix} \tag{3.15}$$

$$= \begin{pmatrix} \frac{x-1}{x+1} & 2\sqrt{\frac{1}{x+1}}\sqrt{\frac{x}{x+1}} \\ 2\sqrt{\frac{1}{x+1}}\sqrt{\frac{x}{x+1}} & -\frac{x-1}{x+1} \end{pmatrix} = \begin{pmatrix} \frac{x-1}{x+1} & \frac{2\sqrt{x}}{x+1} \\ \frac{2\sqrt{x}}{x+1} & -\frac{x-1}{x+1} \end{pmatrix}.$$

Here the new parameter x is introduced. The relation between old and new parametrization of the central transformation is

$$x = (\sqrt{d_2+1} + \sqrt{d_2})^2. \tag{3.16}$$

We introduce the transformation M in the coordinate basis. M represents the coordinate transformation

$$M = T_{12}(d_1)T_{23}(x) \tag{3.17}$$
$$= \begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{\frac{x}{1+x}} & \sqrt{\frac{1}{1+x}} \\ 0 & \sqrt{\frac{1}{1+x}} & -\sqrt{\frac{x}{1+x}} \end{pmatrix}.$$

In the HO basis the representation of M is

$$M_{HO} = \langle((e_1 l_1, e_2 l_2) l_{12}, e_3 l_3) l | T_{12}(d_1)T_{23}(x) | ((e_1' l_1', e_2' l_2') l_{12}', e_3' l_3') l \rangle_{d_1 x} = \tag{3.18}$$
$$\sum_{\substack{\varepsilon_1 \lambda_1, \varepsilon_2 \lambda_2, \Lambda_{23} \\ \varepsilon_2' \lambda_2'}} \langle e_1 l_1, e_2 l_2 : L_{12} | e_1' l_1', \varepsilon_2 \lambda_2 : L_{12} \rangle_{d_1} \delta_{L_{12} e_3 l_3, L_{12}' e_3' l_3'}$$
$$\times \begin{bmatrix} l_1' & 0 & l_1' \\ \lambda_2 & l_3 & \Lambda_{23} \\ L_{12} & l_3 & L \end{bmatrix} \langle \varepsilon_2 \lambda_2, e_3 l_3 : \Lambda_{23} | e_2' l_2', e_3' l_3' : \Lambda_{23} \rangle_x \begin{bmatrix} l_1' & l_2' & L_{12}' \\ 0 & l_3' & l_3' \\ l_1' & \Lambda_{23} & L \end{bmatrix}$$
$$\times \delta_{L_{12}, L_{12}'}$$

and an additional phase matrix F is needed to represent the central diagonal matrix from coordinate basis

$$\langle((e_1 l_1, e_2 l_2) l_{12}, e_3 l_3) l | F | ((e_1' l_1', e_2' l_2') l_{12}', e_3' l_3') l \rangle = (-1)^{e_2} \delta_{e_1 l_1 l_{12} e_3 l_3 l, e_1' l_1' l_{12}' e_3' l_3' l'}. \tag{3.19}$$

The full 4HOB transformation is calculated as

$$4HOB = M_{HO} F M_{HO}^T. \tag{3.20}$$

This simplification allows a significant reduction of the computational efforts which will be presented in the next subsection.

3.1.2 Computation of 4HOBs

In this section, we present the calculation techniques for the harmonic oscillator brackets. These brackets are applicable for three Jacobi coordinates (4HOB). This type of general transformation involves the four particles. Various approaches for calculation of

the 4HOB matrix can be applied depending on a way this transformation is employed in calculations. The computational strategies for 4HOBs allow us to choose a smart approach for higher-order transformations of this type. One has to evaluate the calculation time, as well as memory requirements. All approaches must yield the same result.

A key ingredient for a 4HOB recipe is the TMB which was presented in section 1.5. The use of binomial and trinomial coefficients allows to avoid the costly 6j symbol evaluation using the expressions dependending from the factorials [46]. However, at $E = 28$ the 3HOB begins to produce significant errors due to the large amount of the double precission arithmetic. One of the possible solutions is to change the double precision floating point format calculations into a quandruple precision floating point format. The quadruple precision allows the use of mantissa twice as large (approximately 34 decimal digits) than double precision and thus we get more precise calculations. The next step would be to employ the arbitrary precision libraries. These libraries allow to vary the size of mantissa as the user wants. For quadruple precision one can use the GNU fortran libquadmath [66], while for arbitrary precision the library FMLib [67] can be employed. By using the quadruple precision we were able to extend the calculation of 3HOBs to the HO energy quanta $E = 52$ while sustaining the tolerable margin of error. For precision you must pay with something, and in this case you pay with time. The developed code was paralellized using MPI extensions and tested on a computer cluster Triolith[68]. The calculations results are presented in the tbl.(3.1) and tbl.(3.2). The usage of arbitrary precision allows to extend the range of HO energy quanta from 28 to 43. The downside is that needed resources and time usage are safistactory only for one time calculation. For example, to build up the database for the orbital matrix elements. After building the database of matrix elements one has to solve the efficient access problem. The pre-calculated matrix elements must be reached faster than they can be calculated. The same trends are noticeable for the calculation of the 4HOB matrix elements as well. Usage of extended precision is not feasible if it is used directly in the CFP calculation code as the computation of matrix elements becomes very expensive.

Table 3.1: Calculation time for the 3HOB matrices. E means HO energy; L is angular momentum;DP, QD, FM are the precisions of the calculation in cases of double, quadruple and arbitrary precisions correspondingly. 35 decimal digits of mantissa wee used for the arbitrary precision (FM) code. The mantissa of the quandruple precision is approximately 34 decimal digits. Calculations were performed with supercomputer Triolith [68] using 2 nodes (32 cores of Intel Xeon 'Sandy Bridge' processors at 2.2 Ghz. 10 Gb per node for DP and QD calculation and 20 Gb of RAM per node for the FM.

E	L	Dim	DP	QP	FM
21	11	252	0.11	1.84	91.47
22	8	324	0.35	5.61	117.07
23	9	360	0.46	7.55	362.05
24	8	405	0.74	12.04	629.87
25	9	450	1.09	17.82	231.48
26	10	495	1.47	23.92	507.52
27	9	550	2.46	40.75	416.35
28	10	605	3.3	54.45	835.85
29	11	660	-	69.49	704.42
30	10	726	-	114.65	1345.96
31	11	792	-	148.1	1394.63
32	12	858	-	187.77	1770.32
33	11	936	-	283.22	2837.99
34	12	1014	-	359.45	3268.86
35	13	1092	-	466.97	4267.33
36	12	1183	-	665.26	6273.88
37	13	1274	-	882.41	8064.85
38	12	1365	-	1043.07	10922.75
39	13	1470	-	1588.02	14535.78
40	14	1575	-	1907.75	17475.28
41	13	1680	-	2398.79	25258.89
42	14	1800	-	3070.97	27964.97

Table 3.2: Calculation time (in seconds) for the 4HOB matrices. E means HO energy; L is angular momentum; DP, QD, FM are the precisions of the calculation in cases of double, quadruple and arbitrary precisions correspondingly. 50 decimal digits of mantissa wee used for the arbitrary precision (FM) code. The mantissa of the quandruple precision is approximately 34 decimal digits. Calculations were performed with supercomputer Triolith[68] using 2 nodes (32 cores of Intel Xeon 'Sandy Bridge' processors at 2.2 Ghz. 10 Gb per node for HO energy in range [2,10). 8 nodes and 10 Gb of RAM per node in range [10,14].

E	L	Dim	DP	QD	FM
2	0	6	0.01	0.11	0.11
3	1	18	0.01	0.48	0.21
4	2	36	0.01	0.12	0.49
5	1	63	0.02	0.16	1.37
6	2	125	0.07	0.39	7.67
7	3	207	0.33	1.43	35.27
8	2	330	1.44	6.13	165.08
9	3	542	6.4	27.66	674.27
10	4	804	5.94	91.1	343.24
11	3	1197	23.12	363.94	1374.8
12	4	1764	80.88	1270.49	4497.28
13	5	2436	228.17	3611.29	12916.47
14	4	3444	424.04	6738.47	45540.17

For serial calculation of the 4HOB, the four techniques were used to calculate the matrix elements:

1. Standard 4HOB - The standard matrix element calculation with the full summation over the intermediate variables.

2. M - The 4HOB transformation is calculated with the factorization of the transformation $T_{23}(d_2)$.

3. Ms - The 4HOB transformation is calculated with the factorization of the transformation $T_{23}(d_2)$. Factorization is done in the basis vector consistent with a transformation $T_{23}(d_2)$.

4. mat - The matrix multiplication approach. In this approach, the factorization of the transformation $T_{23}(d_2)$ is done in

Table 3.3: 4HOB calculation time (in seconds) for different types of the realizations for the matrix.

E	L	Dim	$4HOB$	M	Ms	mat	alg
4	2	36	0.064	0.013	0.009	0.001	0.010
5	2	45	0.196	0.022	0.0169	0.002	0.017
6	3	82	1.037	0.097	0.067	0.009	0.071
7	3	207	11.344	0.863	0.582	0.113	0.599
8	4	309	40.795	2.399	1.636	0.483	1.588
9	4	414	132.807	6.287	3.888	1.132	3.757
10	5	591	403.358	15.459	9.442	3.188	8.875
11	5	1116	2402.431	76.252	47.570	20.805	41.802
12	6	1478	6141.757	158.028	98.783	47.573	84.243
13	6	1953	17921.293	392.978	226.357	109.878	191.324

the basis vector consistent with the transformation $T_{23}(d_2)$.

5. alg - Special version of 4HOB transformation with the transformation $T_{23}(0)$. This is a huge simplification for the calculations as the transformation $T_{23}(0)$ has a simpler algebraic expression. One can sum over the recoupling coefficients using the technique in subsection 2.2.2.

The correctness of the results was tested in the interval of HO energy quanta $[4, 13]$, with all corresponding angular momenta values in the interval $[E, E-2, E-4, ...0]$. The speed of calculation compared for the HO energy quanta in the interval $[4, 13]$, with the angular momenta value equal to half of the HO energy value. This was done, to acquire maximal or close to the maximal dimension of the matrix for the HO energy quanta.

The standard matrix element evaluation is not as efficient compared to the other realizations. The calculation times (fig.(3.3)) show the clear advantage of the matrix multiplication technique. The mat approach allows us to speed up the calculations of the matrix by order of two compared to the standard 4HOB. However, since the matrix allocation is very expensive (if the matrices are not stored using sparse matrix techniques), the calculation using the matrix multiplication can have a huge toll on the RAM of the system. One has to investigate the sparsity of the calculated ma-

trices and if possible use sparse matrix techniques for storage.

The parallelism of the 4HOB calculation

In the previous section, it was shown that the calculation of the 4HOB transformation is expensive. One of the obvious solutions to this problem is the parallelization of the computer code. While not dwelling into GPU calculation, which found popularity in recent years, with the rise of the OpenCL and the CUDA techniques one is left with two popular approaches: the OpenMP and the MPI. While the use of the GPUs can be highly effective for the linear algebra operations, the obvious disadvantage is the transferability of the computer code. Ensuring that the code runs on different kinds of computer systems (e.g. different computer clusters) can be difficult if the proprietary compilators (e.g. CUDA) or computational environments are used. It can sometimes require a complete rewrite of the code or maintaining different branches of the solutions for the same problem. The solutions for computation using the OpenMP/MPI are mature for C/C++ or the Fortran programming languages. Fortran programing language is modern (the last revision of the language- Fortran 2018, coming out on November 28th of 2018) and simple enough to implement scientific computing solutions. The main advantage over C/C++ is not having to deal with low-level memory objects as the working with the multidimensional arrays is very convenient in Fortran. Also, as a rule in general, if the C/C++ is supported by the computer system, Fortran will be also supported. This applies also to computational libraries.

3.2 Brackets for four Jacobi coordinates

In this section, the derivation and the expressions for the harmonic oscillator transformation brackets for four Jacobi coordinates (5HOB) are presented. The 5HOBs are involved when the transformation involves the coordinates of five particles. We start from the definition of the five particle wavefunction in intrinsic (Jacobi) coordinates $\boldsymbol{\rho_n}$ with coupled momenta as

$$\{\{\{\{\phi_{e_1l_1}(\boldsymbol{\rho}_1)\otimes\phi_{e_2l_2}(\boldsymbol{\rho}_2)\}_{L_{12}}\otimes\phi_{e_3l_3}(\boldsymbol{\rho}_3)\}_{L_{123}}\}\otimes\phi_{e_4l_4}(\boldsymbol{\rho}_4)\}_{LM}= \tag{3.21}$$

$$\sum_{m_1m_2M_{12}m_3M_{123}m_4} C^{L_{12}M_{12}}_{l_1m_1l_2m_2}C^{L_{123}M_{123}}_{L_{12}M_{12}l_3m_3}C^{LM}_{L_{123}M_{123}l_4m_4}\phi_{e_1l_1m_1}(\boldsymbol{\rho}_1)$$
$$\times\,\phi_{e_2l_2m_2}(\boldsymbol{\rho}_2)\phi_{e_3l_3m_3}(\boldsymbol{\rho}_3)\phi_{e_4l_4m_4}(\boldsymbol{\rho}_4).$$

$\phi_{e_xl_xm_x}(\boldsymbol{\rho}_x)$ is the HO function defined as

$$\phi_{elm}(\boldsymbol{\rho})=(-1)^n\left[\frac{2\,(n!)}{\Gamma\,(n+l+3/2)}\right]^{\frac{1}{2}}e^{\left(-\rho^2/2\right)}\rho^l L_n^{(l+1/2)}\left(\rho^2\right)Y_{lm}\left(\boldsymbol{\rho}/\rho\right). \tag{3.22}$$

The momenta are coupled using CGs marked as C. There are other two ways to couple individual functions to produce the wave function of the four Jacobi coordinates.

In the first case, as in the 4HOB basis vector, we start from the coupling of the first and the second particle angular momenta into the momentum L_{12}. The third and the fourth particle angular momenta are coupled to produce the momentum L_{34}. Then the momenta L_{12} and L_{34} are coupled to produce the total angular momentum of the five particle system L:

$$\left\{\{\phi_{e_1l_1}(\boldsymbol{\rho}_1)\otimes\phi_{e_2l_2}(\boldsymbol{\rho}_2)\}_{L_{12}}\otimes\{\phi_{e_3l_3}(\boldsymbol{\rho}_3)\otimes\phi_{e_4l_4}(\boldsymbol{\rho}_4)\}_{L_{34}}\right\}_{LM}=$$
$$\sum_{\substack{m_1m_2m_3\\m_4M_{12}M_{34}}} C^{L_{12}M_{12}}_{l_1m_1l_2m_2}C^{L_{34}M_{34}}_{l_3m_3l_4m_4}C^{LM}_{L_{12}M_{12}L_{34}M_{34}} \tag{3.23}$$
$$\times\,\phi_{e_1l_1m_1}(\boldsymbol{\rho}_1)\phi_{e_2l_2m_2}(\boldsymbol{\rho}_2)\phi_{e_3l_3m_3}(\boldsymbol{\rho}_3)\phi_{e_4l_4m_4}(\boldsymbol{\rho}_4).$$

In the second case, we first couple the second and the third particle angular momenta to momenta L_{23}. After that we couple the first particle angular momentum l_1 with momentum L_{23} to get the angular momentum of the system of the first three-particles L_{123}. At last, the momentum L_{123} is coupled with the fourth particle angular momentum l_4 to the angular momentum L of five particle

system:

$$\{\{\{\phi_{e_1l_1}(\boldsymbol{\rho}_1)\otimes\{\phi_{e_2l_2}(\boldsymbol{\rho}_2)\otimes\phi_{e_3l_3}(\boldsymbol{\rho}_3)\}_{L_{23}}\}_{L_{123}}\}\otimes\phi_{e_4l_4}(\boldsymbol{\rho}_4)\}_{LM}= \sum_{\substack{m_1m_2m_3\\ m_4M_{23}M_{123}}} C^{L_{23}M_{23}}_{l_2m_2l_3m_3}C^{L_{123}M_{123}}_{l_1m_1L_{23}M_{23}}C^{LM}_{L_{123}M_{123}l_4m_4} \times\phi_{e_1l_1m_1}(\boldsymbol{\rho}_1)\phi_{e_2l_2m_2}(\boldsymbol{\rho}_2)\phi_{e_3l_3m_3}(\boldsymbol{\rho}_3)\phi_{e_4l_4m_4}(\boldsymbol{\rho}_4). \tag{3.24}$$

The coupling schemes in eqs.(3.23,3.24) can be expressed through the coupling scheme from eq.(3.21) similarly using RECs as in the eq.(1.68):

$$|\{\{\{\{\phi_{e_1l_1}(\boldsymbol{\rho}_1)\otimes\phi_{e_2l_2}(\boldsymbol{\rho}_2)\}_{L_{12}}\otimes\phi_{e_3l_3}(\boldsymbol{\rho}_3)\}_{L_{123}}\}\otimes\phi_{e_4l_4}(\boldsymbol{\rho}_4)\}_{LM}\rangle = \left|\{\{\phi_{e_1l_1}(\boldsymbol{\rho}_1)\otimes\phi_{e_2l_2}(\boldsymbol{\rho}_2)\}_{L_{12}}\otimes\{\phi_{e_3l_3}(\boldsymbol{\rho}_3)\otimes\phi_{e_4l_4}(\boldsymbol{\rho}_4)\}_{L_{34}}\}_{LM}\right\rangle \times\langle((l_1,l_2)L_{12},(l_3,l_4)L_{34})L|(((l_1,l_2)L_{12},l_3)L_{123},l_4)L\rangle \ . \tag{3.25}$$

and

$$|\{\{\{\{\phi_{e_1l_1}(\boldsymbol{\rho}_1)\otimes\phi_{e_2l_2}(\boldsymbol{\rho}_2)\}_{L_{12}}\otimes\phi_{e_3l_3}(\boldsymbol{\rho}_3)\}_{L_{123}}\}\otimes\phi_{e_4l_4}(\boldsymbol{\rho}_4)\}_{LM}\rangle = |\{\{\phi_{e_1l_1}(\boldsymbol{\rho}_1)\otimes\{\phi_{e_2l_2}(\boldsymbol{\rho}_2)\otimes\phi_{e_3l_3}(\boldsymbol{\rho}_3)\}_{L_{23}}\}_{L_{123}}\otimes\phi_{e_4l_4}(\boldsymbol{\rho}_4)\}_{LM}\rangle \times\langle(((l_1,(l_2,l_3)L_{23})L_{123},l_4)L|(((l_1,l_2)L_{12},l_3)L_{123},l_4)L\rangle\,. \tag{3.26}$$

The RECs in eqs.(3.25,3.26) are defined through the 6j symbols using the technique presented in section 1.4

$$\langle(((l_1,l_2)L_{12},l_3)L_{123},l_4)L|((l_1,l_2)L_{12},(l_3,l_4)L_{34})L\rangle = \begin{bmatrix} L_{12} & 0 & L_{12}\\ l_3 & l_4 & L_{123}\\ L_{123} & l_4 & L\end{bmatrix} \tag{3.27}$$

$$= (-1)^{L_{12}+l_3+l_4+L}\sqrt{(2L_{123}+1)(2L_{34}+1)}\begin{Bmatrix} L_{12} & l_3 & L_{123}\\ l_4 & L & L_{34}\end{Bmatrix}$$

and

$$\langle(((l_1,l_2)L_{12},l_3)L_{123},l_4)L|((l_1,(l_2l_3)L_{23})L_{123},l_4)L\rangle = \left[\begin{array}{ccc} l_1 & 0 & l_1 \\ l_2 & l_3 & L_{23} \\ L_{12} & l_3 & L \end{array}\right] \tag{3.28}$$
$$= (-1)^{l_1+l_2+l_3+L_{123}}\sqrt{(2L_{12}+1)(2L_{23}+1)}\left\{\begin{array}{ccc} l_1 & l_2 & L_{12} \\ l_3 & L_{123} & L_{23} \end{array}\right\}.$$

We will start the derivation of 5HOB in the basis vector from eq.(3.24). The 5HOBs are defined as the five-particle coordinate transformation from one set to another

$$\begin{aligned}\{\{\{\{e_1l_1(\boldsymbol{\rho}_1),e_2l_2(\boldsymbol{\rho}_2)\}L_{12},e_3l_3(\boldsymbol{\rho}_3)\}\,L_{123},e_4l_4(\boldsymbol{\rho}_4)\}LM\} = \\ \sum_{\substack{e_1'l_1'e_2'l_2'L_{12}' \\ e_3'l_3'L_{123}'e_4'l_4'}} \langle\{\{\{e_1l_1,e_2l_2\}L_{12},e_3l_3\}\,L_{123},e_4l_4\}LM| \\ \times\{\{e_1'l_1',e_2'l_2'\}L_{12}',e_3'l_3'L_{123}',e_4'l_4'\}LM\rangle_{d_1d_2d_3} \\ \times\{\{\{\{e_1'l_1'(\boldsymbol{\rho}_1'),e_2'l_2'(\boldsymbol{\rho}_2')\}L_{12}',e_3'l_3'(\boldsymbol{\rho}_3')\}\,L_{123},\}\,e_4'l_4'(\boldsymbol{\rho}_4')\}LM\}\,.\end{aligned} \tag{3.29}$$

The total oscillator energy on both sides of the brackets $e_1+e_2+e_3+e_4 = e_1'+e_2'+e_3'+e_4'$ must be conserved. The angular momentum coupling must obey the triangular rules.

Firstly, let us consider 5HOB transformation in the coordinate basis. The 5HOB is the SO_4 coordinate transformation represented by 4×4 matrix. This matrix can be expressed using a similar technique presented in section 3.1 for the three Jacobi coordinate transformation. For the four Jacobi coordinate transformation instead of the three two-dimensional coordinate transformations we get five

$$\begin{pmatrix} \boldsymbol{\rho}_1 \\ \boldsymbol{\rho}_2 \\ \boldsymbol{\rho}_3 \\ \boldsymbol{\rho}_4 \end{pmatrix} = T_{12}(d_1)T_{23}(d_2)T_{34}(d_3)T_{23}(d_2)T_{12}(d_1) \begin{pmatrix} \boldsymbol{\rho}'_1 \\ \boldsymbol{\rho}'_2 \\ \boldsymbol{\rho}'_3 \\ \boldsymbol{\rho}'_4 \end{pmatrix}$$

$$\begin{pmatrix} \boldsymbol{\rho}_1 \\ \boldsymbol{\rho}_2 \\ \boldsymbol{\rho}_3 \\ \boldsymbol{\rho}_4 \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{d_2}{1+d_2}} & \sqrt{\frac{1}{1+d2}} & 0 \\ 0 & \sqrt{\frac{1}{1+d_2}} & -\sqrt{\frac{d_2}{1+d_2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{d_3}{1+d_3}} & \sqrt{\frac{1}{1+d_3}} \\ 0 & 0 & \sqrt{\frac{1}{1+d_3}} & -\sqrt{\frac{d_3}{1+d_3}} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{d_2}{1+d_2}} & \sqrt{\frac{1}{1+d_2}} & 0 \\ 0 & \sqrt{\frac{1}{1+d_2}} & -\sqrt{\frac{d_2}{1+d_2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{3.30}$$

$$\times \begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{\rho}'_1 \\ \boldsymbol{\rho}'_2 \\ \boldsymbol{\rho}'_3 \\ \boldsymbol{\rho}'_4 \end{pmatrix}.$$

This coordinate transformation is parametrized by the three variables d_1, d_2, d_3, known as the mass-ratio parameters [60]. They act as the Euler angles and depend on the Jacobi tree. The relations between the Euler angles and the mass-ratio parameter d is

$$\sin(\alpha) = \sqrt{\frac{d}{1+d}} \tag{3.31}$$

or

$$\cos(\alpha) = \sqrt{\frac{1}{1+d}} \tag{3.32}$$

The relations in the eq.(3.31) and eq.(3.32) allow calculating the additional phase multipliers required for the representation of the

transposition operators using the 5HOBs. Each of the five transformation matrices is an orthogonal two-particle coordinate transformation described in section 1.5.

We follow the same pattern as in the 4HOB coordinate transformation described in subsection 3.1.1. The matrix representing the transformation $T_{34}(d_3)$ is split into the product of the three matrices

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{d_3}{1+d_3}} & \sqrt{\frac{1}{1+d_3}} \\ 0 & 0 & \sqrt{\frac{1}{1+d_3}} & -\sqrt{\frac{d_3}{1+d_3}} \end{pmatrix} = \tag{3.33}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{x}{1+x}} & \sqrt{\frac{1}{1+x}} \\ 0 & 0 & \sqrt{\frac{1}{1+x}} & -\sqrt{\frac{x}{1+x}} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{x}{1+x}} & \sqrt{\frac{1}{1+x}} \\ 0 & 0 & \sqrt{\frac{1}{1+x}} & -\sqrt{\frac{x}{1+x}} \end{pmatrix},$$

with a newly introduced mass-ratio parameter $x = (\sqrt{d_3+1} + \sqrt{d_3})^2$. The factorization of the matrix A can be understood as the reformulation of the transformation as the eigenvalue problem. The diagonalized matrix A has the eigenvalues $\{1, 1, 1, -1\}$ and the associated eigenvectors are given by the matrix

$$V = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{x}{1+x}} & \sqrt{\frac{1}{1+x}} \\ 0 & 0 & \sqrt{\frac{1}{1+x}} & -\sqrt{\frac{x}{1+x}} \end{pmatrix}. \tag{3.34}$$

Let us denote the product of the three transformations $T_{12}(d_1)\, T_{23}(d_2)\, T_{34}(x)$ as S :

$$S = T_{12}\left(d_1\right) T_{23}\left(d_2\right) T_{34}\left(x\right) = \begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$
$$\times \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{d_2}{1+d_2}} & \sqrt{\frac{1}{1+d_2}} & 0 \\ 0 & \sqrt{\frac{1}{1+d_2}} & -\sqrt{\frac{d_2}{1+d_2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{x}{1+x}} & \sqrt{\frac{1}{1+x}} \\ 0 & 0 & \sqrt{\frac{1}{1+x}} & -\sqrt{\frac{x}{1+x}} \end{pmatrix}. \tag{3.35}$$

Then the coordinate transformation of the four Jacobi coordinates from eq.(3.30) can be redefined as:

$$\begin{pmatrix} \boldsymbol{\rho}_1 \\ \boldsymbol{\rho}_2 \\ \boldsymbol{\rho}_3 \\ \boldsymbol{\rho}_4 \end{pmatrix} = S \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} S^T \begin{pmatrix} \boldsymbol{\rho}'_1 \\ \boldsymbol{\rho}'_2 \\ \boldsymbol{\rho}'_3 \\ \boldsymbol{\rho}'_4 \end{pmatrix}. \tag{3.36}$$

S^T is the transpose of the matrix S. The transformations of state vectors induced by the matrix S will be used for the derivation of the brackets. First step is the derivation of the matrix elements for the transformations $T_{12}\left(d_1\right) T_{23}\left(d_2\right)$. It will change the initial basis vector, denoted as:

$$|\alpha\rangle = |(((e_1 l_1, e_2 l_2) L_{12}, e_3 l_3) L_{123}\rangle \tag{3.37}$$

to the basis vector

$$|\alpha'\rangle = |(((e'_1 l'_1, e'_2 l'_2) L'_{12}, e'_3 l'_3) L'_{123}\rangle. \tag{3.38}$$

The transformation $T_{12}\left(d_1\right) T_{23}\left(d_2\right)$ is expressed as a sum through:

$$\begin{aligned} &\langle\alpha|T_{12}(d_1)T_{23}(d_2)|\alpha'\rangle \\ &= \sum_{\beta} \langle\alpha|T_{12}(d_1)|\beta\rangle\langle\beta|T_{23}(d_2)|\alpha'\rangle, \end{aligned} \tag{3.39}$$

where β denotes intermediate states

$$|\beta\rangle = |(((\varepsilon_1\lambda_1, \varepsilon_2\lambda_2)\Lambda_{12}, \varepsilon_3\lambda_3)\Lambda_{123}\rangle. \tag{3.40}$$

ε_i denotes the HO energy, λ_i are the angular momenta corresponding to ε_i $(i = 1, ..., 4)$; Λ_j $(j = 12, 123)$ and Λ mark the coupled angular momenta. In the eq.(3.39) the transformation $T_{12}(d_1)$ transforms only the Jacobi coordinates $\boldsymbol{\rho}_1, \boldsymbol{\rho}_2$ and acts on the corresponding basis states with quantum numbers $e_1 l_1, e_2 l_2$:

$$\begin{aligned} &\langle(((e_1 l_1, e_2 l_2)L_{12}, e_3 l_3)L_{123}, e_4 l_4)L|T_{12}(d_1) \\ &\times|(((\varepsilon_1\lambda_1, \varepsilon_2\lambda_2)\Lambda_{12}, \varepsilon_3\lambda_3)\Lambda_{123}, \varepsilon_4\lambda_4)\Lambda\rangle \\ &= \langle e_1 l_1, e_2 l_2 : L_{12}\,|\varepsilon_1\lambda_1, \varepsilon_2\lambda_2 : L_{12}\rangle_{d_1}\, \delta_{L_{12}e_3 l_3 L_{123} e_4 l_4 L, \Lambda_{12}\varepsilon_3\lambda_3\Lambda_{123} e_4' l_4' L'}. \end{aligned} \tag{3.41}$$

The transformation results in Talmi- Moshinsky brackets [13] with the mass ratio parameter d_1 and the Dirac delta functions δ for unchanged quantum numbers. The next transformation is provided with the operator $T_{23}(d_2)$, which transforms the coordinates $\boldsymbol{\rho}_2, \boldsymbol{\rho}_3$. In this case we first have to change the coupling scheme from

$$\{\{\phi_{e_1 l_1}(\boldsymbol{\rho}_1) \otimes \phi_{e_2 l_2}(\boldsymbol{\rho}_2)\}_{L_{12}} \otimes \phi_{e_3 l_3}(\boldsymbol{\rho}_3)\}_{L_{123}} \tag{3.42}$$

to

$$\{\{\phi_{e_1 l_1}(\boldsymbol{\rho}_1) \otimes \{\phi_{e_2 l_2}(\boldsymbol{\rho}_2) \otimes \phi_{e_3 l_3}(\boldsymbol{\rho}_3)\}_{L_{23}}\}_{L_{123}} \tag{3.43}$$

and then transform the variables:

$$\begin{aligned} &\langle(((\varepsilon_1\lambda_1, \varepsilon_2\lambda_2)\Lambda_{12}, \varepsilon_3\lambda_3)\Lambda_{123}, \varepsilon_4\lambda_4)\Lambda|T_{23}(d_2) \\ &\times|(((e_1 l_1, e_2 l_2)L_{12}, e_3 l_3)L_{123}, e_4 l_4)L\rangle = \\ &\sum_{\Lambda_{23}} \langle(((\lambda_1, \lambda_2)\Lambda_{12}, \lambda_3)\Lambda_{123}, \lambda_4)\Lambda|(((\lambda_1, (\lambda_2, \lambda_3)\Lambda_{23})\Lambda_{123}, \lambda_4)\Lambda\rangle \\ &\times\langle\varepsilon_2\lambda_2, e_3 l_3 : \Lambda_{23}|e_2' l_2', e_3' l_3' : \Lambda_{23}\rangle_{d_2} \\ &\times\left\langle(((l_1', (l_2', l_3')\Lambda_{23})L_{123}', l_4')L'|(((l_1', l_2')L_{12}', l_3')L_{123}', l_4')L'\right\rangle \\ &\times\delta_{\varepsilon_1\lambda_1\Lambda_{12}\Lambda_{123}\varepsilon_4\lambda_4\Lambda, e_1' l_1' L_{12}' L_{123}' e_4' l_4' L'}. \end{aligned} \tag{3.44}$$

We need to introduce a new sum, running through the new angular momentum quantum number Λ_{23}. The result is the Talmi-

Moshinsky bracket with mass ratio parameter d_2, Dirac delta functions δ and two RECs. We rewrite the expression of the transposition from eq.(3.39) by taking into account the Dirac delta functions from eq.(3.41) and eq.(3.44)

$$\begin{aligned}
&\langle(((e_1l_1,e_2l_2)L_{12},e_3l_3)L_{123},e_4l_4)L|T_{12}(d_1)T_{23}(d_2)\\
&\quad\times|(((e_1'l_1',e_2'l_2')L_{12}',e_3'l_3')L_{123}',e_4'l_4')L'\rangle = \\
&\quad\sum_{\varepsilon_2\lambda_2}\langle e_1l_1,e_2l_2:L_{12}\,|e_1'l_1',\varepsilon_2\lambda_2:L_{12}\rangle_{d_1}\\
\times\sum_{\Lambda_{23}}&\begin{bmatrix} l_1' & 0 & l_1' \\ \lambda_2 & l_3 & \Lambda_{23} \\ L_{12} & l_3 & L_{123}\end{bmatrix}\langle\varepsilon_2\lambda_2,e_3l_3:\Lambda_{23}\,|e_2'l_2',e_3'l_3':\Lambda_{23}\rangle_{d_2}\\
&\times\begin{bmatrix} l_1' & l_2' & L_{12}' \\ 0 & l_3' & l_3' \\ l_1' & \Lambda_{23} & L_{123}'\end{bmatrix}\delta_{L_{123}e_4l_4L,L_{123}'e_4'l_4'L'}.
\end{aligned}\tag{3.45}$$

The next step is to add the transformation $T_{34}(x)$. To accomplish this, the transformation is expressed though another sum:

$$\begin{aligned}
&\langle\alpha|T_{12}(d_1)T_{23}(d_2)T_{34}(x)|\alpha'\rangle\\
&=\sum_\gamma\langle\alpha|T_{12}(d_1)T_{23}(d_2)|\gamma\rangle\langle\gamma|T_{34}(x)|\alpha'\rangle,
\end{aligned}\tag{3.46}$$

where the intermediate state $|\gamma\rangle$ equals to

$$|\gamma\rangle = |(((\varepsilon_1'\lambda_1^{'},\varepsilon_2'\lambda_2')\Lambda_{12}',\varepsilon_3'\lambda_3')\Lambda_{123}',\varepsilon_4'\lambda_4')\Lambda'\rangle.\tag{3.47}$$

$T_{34}(x)$ transforms only the coordinates ρ_3,ρ_4 and the corresponding basis states with quantum numbers e_3l_3,e_4l_4. To transform the variables, the coupling scheme

$$\{\{\{\{\phi_{e_1l_1}(\boldsymbol{\rho}_1)\otimes\phi_{e_2l_2}(\boldsymbol{\rho}_2)\}_{L_{12}}\otimes\phi_{e_3l_3}(\boldsymbol{\rho}_3)\}_{L_{123}}\}\otimes\phi_{e_4l_4}(\boldsymbol{\rho}_4)\}_{LM}\tag{3.48}$$

is changed to

$$\big\{\{\phi_{e_1l_1}(\boldsymbol{\rho}_1)\otimes\phi_{e_2l_2}(\boldsymbol{\rho}_2)\}_{L_{12}}\otimes\{\phi_{e_3l_3}(\boldsymbol{\rho}_3)\otimes\phi_{e_4l_4}(\boldsymbol{\rho}_4)\}_{L_{34}}\big\}_{LM}\tag{3.49}$$

with help of the recoupling coefficient:

$$\begin{aligned}
&\langle(((\varepsilon_1'\lambda_1^{'},\varepsilon_2'\lambda_2')\Lambda_{12}',\varepsilon_3'\lambda_3')\Lambda_{123}',\varepsilon_4'\lambda_4')\Lambda'|T_{34}(x)\\
&\times|(((e_1'l_1',e_2'l_2')L_{12}',e_3'l_3')L_{123}',e_4'l_4')L'\rangle\\
=\sum_{\Lambda_{34}'}&\begin{bmatrix}\Lambda_{12}^{'} & 0 & \Lambda_{12}^{'}\\ \lambda_3' & \lambda_4' & \Lambda_{34}'\\ \Lambda_{123}^{'} & \lambda_4' & \Lambda^{'}\end{bmatrix}\langle\varepsilon_3'\lambda_3',e_4l_4:\Lambda_{34}'|e_3'l_3',e_4'l_4':\Lambda_{34}'\rangle_x \quad (3.50)\\
&\times\begin{bmatrix}L_{12}' & l_3' & L_{123}'\\ 0 & l_4' & l_4'\\ L_{12}' & \Lambda_{34}' & L'\end{bmatrix}\delta_{\varepsilon_1'\lambda_1'\Lambda_{12}'\varepsilon_2'\lambda_2'\Lambda_{123}'\Lambda',e_1'l_1'L_{12}'e_2'l_2'L_{123}'L'}.
\end{aligned}$$

The expression $\langle\alpha|T_{12}(d_1)T_{23}(d_2)|\alpha'\rangle$ must be rewritten in such a way that it conforms to eq.(3.44). As the transformation $T_{34}(x)$ corresponds to quantum numbers e_3l_3, e_4l_4, we have only one summation over $\varepsilon_3'\lambda_3'$ for the transformations $T_{23}(d_2)$ and $T_{34}(x)$. Taking into account the relevant Dirac delta functions δ for $\langle\alpha|T_{12}(d_1)T_{23}(d_2)|\gamma^{'}\rangle$ we get

$$\begin{aligned}
&\langle(((e_1l_1,e_2l_2)L_{12},e_3l_3)L_{123},e_4l_4)L|T_{12}(d_1)T_{23}(d_2)\\
&\times|(((\varepsilon_1'\lambda_1^{'},\varepsilon_2'\lambda_2')\Lambda_{12}',\varepsilon_3'\lambda_3')\Lambda_{123}',\varepsilon_4'\lambda_4')\Lambda'\rangle\\
&=\sum_{\varepsilon_2\lambda_2}\langle e_1l_1,e_2l_2:L_{12}\,|e_1'l_1',\varepsilon_2\lambda_2:L_{12}\rangle_{d_1} \quad (3.51)\\
\times\sum_{\Lambda_{23}}&\begin{bmatrix}l_1' & 0 & l_1'\\ \lambda_2 & l_3 & \Lambda_{23}\\ L_{12} & l_3 & L_{123}\end{bmatrix}\langle\varepsilon_2\lambda_2,e_3l_3:\Lambda_{23}\,|e_2'l_2',\varepsilon_3'\lambda_3':\Lambda_{23}\rangle_{d_2}\\
&\times\begin{bmatrix}l_1' & l_2' & L_{12}'\\ 0 & \lambda_3^{'} & \lambda_3^{'}\\ l_1' & \Lambda_{23} & L_{123}'\end{bmatrix}\delta_{L_{123}e_4l_4L,L_{123}'e_4'l_4'L'}.
\end{aligned}$$

For the transformation $\langle\gamma|T_{34}(x)|\alpha'\rangle$ the expression is:

$$\begin{aligned}
&\langle((((\varepsilon_1'\lambda_1^{'},\varepsilon_2'\lambda_2')\Lambda_{12}',\varepsilon_3'\lambda_3')\Lambda_{123}',e_4l_4)\Lambda'|T_{34}(x)\\
&\times|(((e_1'l_1',e_2'l_2')L_{12}',e_3'l_3')L_{123}',e_4'l_4')L'\rangle\\
&=\sum_{\varepsilon_3'\lambda_3'\Lambda_{34}'}\begin{bmatrix} L_{12}^{'} & 0 & L_{12}^{'}\\ \lambda_3' & l_4 & \Lambda_{34}'\\ L_{123}^{'} & l_4 & L\end{bmatrix}\langle\varepsilon_3'\lambda_3',e_4l_4:\Lambda_{34}'|e_3'l_3',e_4'l_4':\Lambda_{34}'\rangle_x \qquad (3.52)\\
&\times\begin{bmatrix} L_{12}' & l_3' & L_{123}'\\ 0 & l_4' & l_4'\\ L_{12}' & \Lambda_{34}' & L'\end{bmatrix}\delta_{\varepsilon_1'\lambda_1'\Lambda_{12}'\varepsilon_2'\lambda_2'\Lambda_{123}'\Lambda',e_1'l_1'L_{12}'e_2'l_2'L_{123}'L'}.
\end{aligned}$$

The coordinate transformation S, eq.(3.35) induces the five particle state vector transformation in the HO basis with the operator $S_{HO}=T_{12}(d_1)T_{23}(d_2)T_{34}(x)$:

$$\langle((((e_1l_1,e_2l_2)L_{12},e_3l_3)L_{123},e_4l_4)L|S_{HO}|(((e_1'l_1',e_2'l_2')L_{12}',e_3'l_3')L_{123}',e_4'l_4')L'\rangle. \qquad (3.53)$$

The matrix elements of the operator S_{HO} are equal to matrix elements corresponding to the two dimensional transformations described in eqs.(3.41, 3.44, 3.2):

$$\begin{aligned}
&\langle((((e_1l_1,e_2l_2)L_{12},e_3l_3)L_{123},e_4l_4)L|S_{HO}|(((e_1'l_1',e_2'l_2')L_{12}',e_3'l_3')L_{123}',e_4'l_4')L'\rangle=\\
&\sum_{\varepsilon_2\lambda_2}\langle e_1l_1,e_2l_2:L_{12}\,|e_1'l_1',\varepsilon_2\lambda_2:L_{12}\rangle_{d_1}\\
&\times\sum_{\Lambda_{23}}\begin{bmatrix} l_1' & 0 & l_1'\\ \lambda_2 & l_3 & \Lambda_{23}\\ L_{12} & l_3 & L_{123}\end{bmatrix}\langle\varepsilon_2\lambda_2,e_3l_3:\Lambda_{23}\,|e_2'l_2',\varepsilon_3'\lambda_3':\Lambda_{23}\rangle_{d_2}\\
&\times\begin{bmatrix} l_1' & l_2' & L_{12}'\\ 0 & \lambda_3' & l_3'\\ l_1' & \Lambda_{23} & L_{123}'\end{bmatrix}\delta_{L_{123}e_4l_4L,L_{123}'e_4'l_4'L'}\\
&\times\sum_{\varepsilon_3'\lambda_3'\Lambda_{34}'}\begin{bmatrix} L_{12}^{'} & 0 & L_{12}^{'}\\ \lambda_3' & l_4 & \Lambda_{34}'\\ L_{123}^{'} & l_4 & L\end{bmatrix}\langle\varepsilon_3'\lambda_3',e_4l_4:\Lambda_{34}'|e_3'l_3',e_4'l_4':\Lambda_{34}'\rangle_x\\
&\times\begin{bmatrix} L_{12}' & l_3' & L_{123}'\\ 0 & l_4' & l_4'\\ L_{12}' & \Lambda_{34}' & L'\end{bmatrix}\delta_{L,L'}. \qquad (3.54)
\end{aligned}$$

The method presented here does not require the calculation of the full expression of the 5HOB matrix which is quite complicated. Instead of the full 5HOB matrix calculation, it is enough to calculate the 5HOB eigenvector matrix M and the diagonal eigenvalue matrix F in a way, that:

$$5HOB = S_{HO}^{T} F S_{HO}. \tag{3.55}$$

The elements of the matrix F are equal to $(-1)^{e'_4}$ and S_{HO}^{T} is the transpose of matrix S_{HO}.

3.2.1 OFPCs using 5HOBs

In this subsection, we discuss the calculation of the orbital fractional parentage coefficients (OFPCs) using 5HOBs. 5HOBs are useful when the transpositions involve four Jacobi coordinates. The discussion is done using binary cluster formalism.

Systems divided in $N_1 = N - 1$ and $N_2 = 1$

The 5HOBs are applicable for the systems with clusterization $N_1 = N - 1$ and $N_2 = 1$. The first cluster has two intrinsic subclusters, composed of the K and $N-1-K$ particles, respectively. An example of the Jacobi tree for such clusterization is present in fig.(3.1).

In this case, the two-body transposition operator $P_{N_1 N} = P_{N-1N}$ exchanges the last two particles [23]. An example of this case can be an eight-particle system, composed of the two clusters with $N_1 = 7$ and $N_2 = 1$, respectively. Here the first cluster has its own subclusters of $K = 2$ and $N - 1 - K = 5$ particles. The Jacobi tree corresponding to this example is presented in fig.(3.2). The intrinsic Jacobi coordinates of this tree are

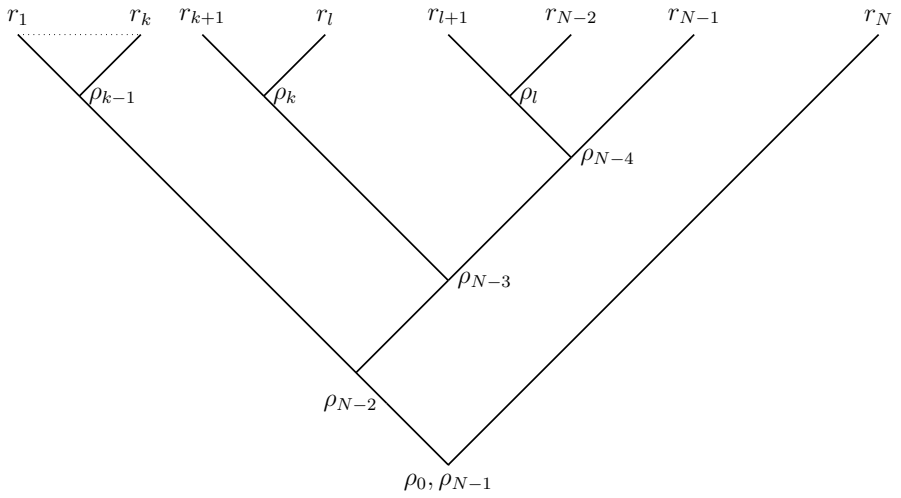


Figure 3.1: Jacobi tree for a N particle system, composed of N_1 and 1 particle, where the N_1 cluster has its own clusterization.

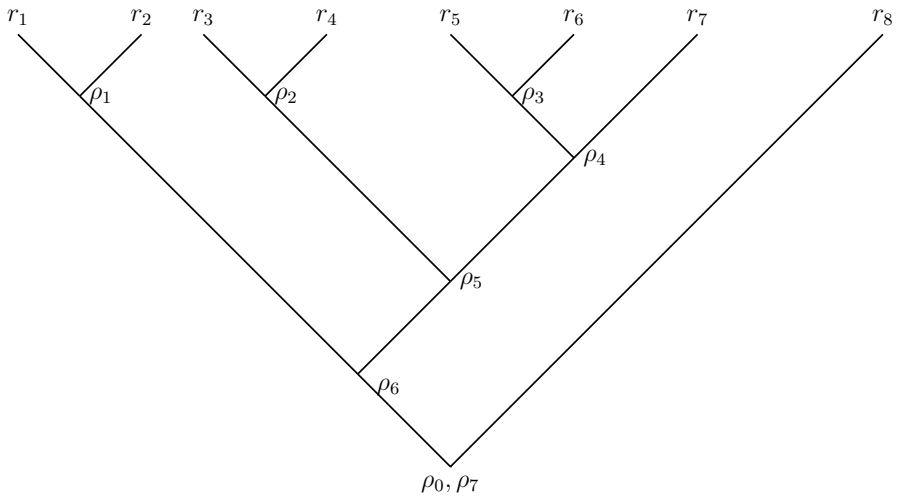


Figure 3.2: Jacobi tree for an eight particle system, composed of $N_1 = 7$ and $N_2 = 1$ particle clusters, where the $N_1 = 7$ cluster has its own clusterization.

$$
\begin{aligned}
\boldsymbol{\rho}_1 &= \frac{1}{\sqrt{2}}\left(\boldsymbol{r}_1 - \boldsymbol{r}_2\right), \\
\boldsymbol{\rho}_2 &= \frac{1}{\sqrt{2}}\left(\boldsymbol{r}_3 - \boldsymbol{r}_4\right), \\
\boldsymbol{\rho}_3 &= \frac{1}{\sqrt{2}}\left(\boldsymbol{r}_5 - \boldsymbol{r}_6\right), \\
\boldsymbol{\rho}_4 &= \sqrt{\frac{1}{6}}\left(\boldsymbol{r}_5 + \boldsymbol{r}_6\right) - \sqrt{\frac{2}{3}}\boldsymbol{r}_7, \\
\boldsymbol{\rho}_5 &= \sqrt{\frac{3}{10}}\left(\boldsymbol{r}_3 + \boldsymbol{r}_4\right) - \sqrt{\frac{2}{15}}\left(\boldsymbol{r}_5 + \boldsymbol{r}_6 + \boldsymbol{r}_7\right) \\
\boldsymbol{\rho}_6 &= \sqrt{\frac{5}{14}}\left(\boldsymbol{r}_1 + \boldsymbol{r}_2\right) - \sqrt{\frac{2}{35}}\left(\boldsymbol{r}_3 + \boldsymbol{r}_4 + \boldsymbol{r}_5 + \boldsymbol{r}_6 + \boldsymbol{r}_7\right) \\
\boldsymbol{\rho}_7 &= \sqrt{\frac{1}{56}}\left(\boldsymbol{r}_1 + \boldsymbol{r}_2 + \boldsymbol{r}_3 + \boldsymbol{r}_4 + \boldsymbol{r}_5 + \boldsymbol{r}_6 + \boldsymbol{r}_7\right) - \sqrt{\frac{7}{8}}\boldsymbol{r}_8
\end{aligned}
\tag{3.56}
$$

where $\mathbf{r}_i$ $(i = 1, ..., 8)$ are the Cartesian coordinates of the particles. The c.m. coordinate is not included as the transposition operator P does not act upon it. The two-body transposition operator in this case is $P_{N-1,N} = P_{78}$. The operator acts on the Cartesian coordinates of the seventh and eight particles only. That means that only four Jacobi coordinates $\rho_i (i = 4, ..., 7)$ are changed. The transformation of the Jacobi coordinates can be written as:

$$\begin{pmatrix} \boldsymbol{\rho}_4 \\ \boldsymbol{\rho}_5 \\ \boldsymbol{\rho}_6 \\ \boldsymbol{\rho}_7 \end{pmatrix} = \begin{pmatrix} -\sqrt{\frac{1}{6}} & \sqrt{\frac{5}{6}} & 0 & 0 \\ \sqrt{\frac{5}{6}} & \sqrt{\frac{1}{6}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{15}} & \sqrt{\frac{14}{15}} & 0 \\ 0 & \sqrt{\frac{14}{15}} & \frac{1}{\sqrt{15}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{3.57}$$

$$\times \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{7} & \frac{4\sqrt{3}}{7} \\ 0 & 0 & \frac{4\sqrt{3}}{7} & -\frac{1}{7} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{15}} & \sqrt{\frac{14}{15}} & 0 \\ 0 & \sqrt{\frac{14}{15}} & \frac{1}{\sqrt{15}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\times \begin{pmatrix} -\sqrt{\frac{1}{6}} & \sqrt{\frac{5}{6}} & 0 & 0 \\ \sqrt{\frac{5}{6}} & \sqrt{\frac{1}{6}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{\rho}'_4 \\ \boldsymbol{\rho}'_5 \\ \boldsymbol{\rho}'_6 \\ \boldsymbol{\rho}'_7 \end{pmatrix}.$$

The mass ratio parameters in this case are $d_1 = \frac{1}{5}$, $d_2 = \frac{1}{14}$ and $d_3 = \frac{1}{48}$.
The transformation matrix of the four Jacobi coordinates presented in eq.(3.57) differs from the expression presented in eq.(3.30) by a multiplier. To calculate the 5HOB according to the formulas presented in eqs.(3.54, 3.55) it is required to multiply the corresponding Talmi- Moshinsky brackets by $(-1)^{l_1+\lambda_3}$.

Systems divided in $N_1 = N - 2$ and $N_2 = 2$

The second example of a 5HOB application is the transformation of Jacobi coordinates of the N particle system for the clusterization scheme $N_1 = N - 2$ and $N_2 = 2$. In this case, the first cluster has two intrinsic subclusters composed of K and $N - 2 - K$ particles, respectively. The two-body transposition operator $P_{N-2,N}$ changes the $N - 2$-th and the $N-$th particles. An example of a Jacobi tree for such clusterization is presented in fig.(3.3). For illustration, we will use a five particle system composed of two clusters with $N_1 = 3$ and $N_2 = 2$ particles respectively. Here the first cluster has the intrinsic clusterization of $K = 1$ and $N - K - 2 = 2$ particles.

The two-body transposition operator equals $P_{N-2,N} = P_{35}$. It acts on the Cartesian coordinates of the third, and the fifth particles only.

A corresponding five particle Jacobi tree for this clusterization is presented in fig.(3.4). The intrinsic Jacobi coordinates of this tree are:

$$\begin{aligned}
\boldsymbol{\rho_1} &= \frac{1}{\sqrt{2}}\left(\boldsymbol{r_2} - \boldsymbol{r_3}\right) \\
\boldsymbol{\rho_2} &= \sqrt{\frac{2}{3}}\boldsymbol{r_1} - \sqrt{\frac{1}{6}}\left(\boldsymbol{r_2} + \boldsymbol{r_3}\right) \\
\boldsymbol{\rho_3} &= \frac{1}{\sqrt{2}}\left(\boldsymbol{r_4} - \boldsymbol{r_5}\right) \\
\boldsymbol{\rho_4} &= \sqrt{\frac{2}{15}}\left(\boldsymbol{r_1} + \boldsymbol{r_2} + \boldsymbol{r_3}\right) - \sqrt{\frac{3}{10}}\left(\boldsymbol{r_4} + \boldsymbol{r_5}\right)
\end{aligned} \tag{3.58}$$

The transposition of the Jacobi coordinates from the eq.(3.30) is

$$\begin{aligned}
\begin{pmatrix} \boldsymbol{\rho_1} \\ \boldsymbol{\rho_2} \\ \boldsymbol{\rho_3} \\ \boldsymbol{\rho_4} \end{pmatrix} = &\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{3}{7}} & \frac{2}{\sqrt{7}} & 0 \\ 0 & \frac{2}{\sqrt{7}} & -\sqrt{\frac{3}{7}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\
&\times \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -\frac{1}{6} & \frac{\sqrt{5\cdot 7}}{6} \\ 0 & 0 & \frac{\sqrt{5\cdot 7}}{6} & \frac{1}{6} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{3}{7}} & \frac{2}{\sqrt{7}} & 0 \\ 0 & \frac{2}{\sqrt{7}} & -\sqrt{\frac{3}{7}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\
&\times \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{\rho'_1} \\ \boldsymbol{\rho'_2} \\ \boldsymbol{\rho'_3} \\ \boldsymbol{\rho'_4} \end{pmatrix}.
\end{aligned} \tag{3.59}$$

The mass ratio parameters in this case are $d_1 = \frac{1}{3}$, $d_2 = \frac{3}{4}$ and $d_3 = \frac{1}{35}$. The transformation matrix of the four Jacobi coordinates presented in eq.(3.59) differs from the expression presented in eq. (3.30) by the location of signs in the first, the third, and the fifth two-dimensional transformation matrices. To calculate the 5HOB

according to formulas presented in eqs. (3.54, 3.55) it is required to multiply the corresponding Talmi-Moshinsky brackets by the phase multiplier $(-1)^{l_1+l_4^{'}+\lambda_2+\lambda_3}$.
The eigenvectors of the 5HOB matrices in these two examples cor-

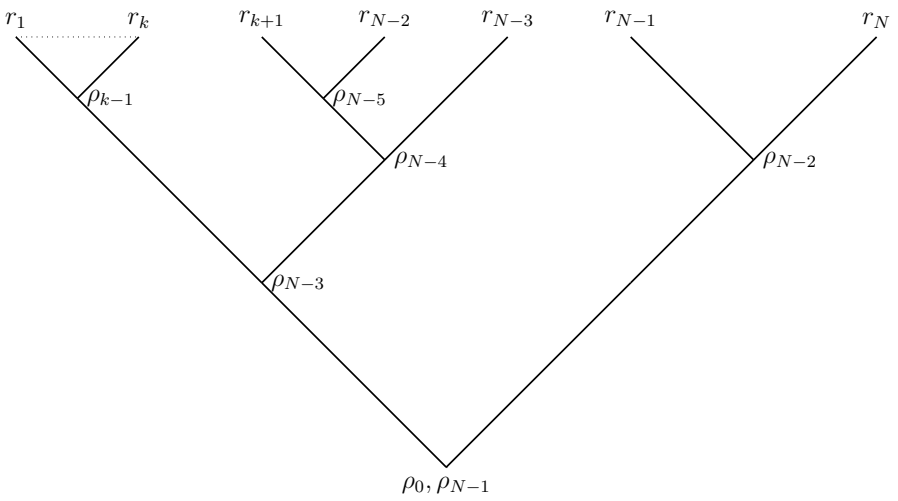


Figure 3.3: Jacobi tree for a N particle system, composed of N_1 and 2 particles, where the first cluster has two intrinsic K and $N-2-K$ particle subclusters

respond to the OFPCs of the described systems if the subclusters are properly antisymmetrized and their OFPCs are known. The antisymmetric subspace can be located according to the Λ formalism described in chapter 1.

In this subsection, we discussed the application of the 5HOB technique for the transposition operator calculation in the HO basis.

3.2.2 Computation of 5HOBs

In this section, we present the details for the computation of the harmonic oscillator transformation brackets for four Jacobi coordinates. The approach for the calculation of the 5HOBs is implemented using the Fortran90 programming language. The high-performance library ScaLAPACK was employed for the parallel linear algebra operations with double precision variables. Calculations

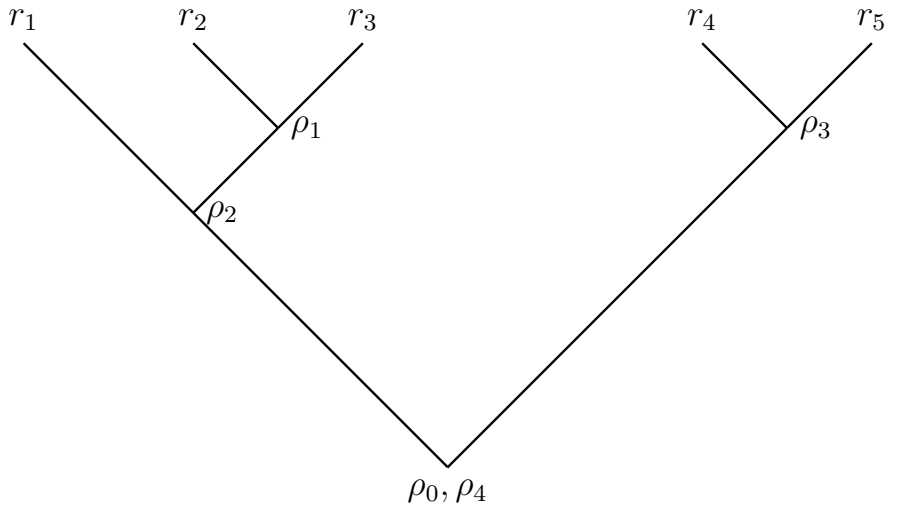


Figure 3.4: Jacobi tree for a five particle system, composed of $N_1 = 3$ and $N_2 = 2$ particle clusters, where the first cluster has its own clusterization of $K = 1$ and $N - K - 2 = 2$ particles

were performed on the HPC "Sauletekis" on three computing nodes, where each node has 12 Intel x86_64 cores and 96 GB of RAM. We tested our method by calculating the 5HOB matrices eq.(3.54), where the sums run over the free parameters $\epsilon_2\lambda_2\epsilon'_3\lambda'_3\Lambda_{23}\Lambda'_{34}$. The calculated matrices represent the operators P_{78} (tbl.3.4) and P_{35} (tbl.3.5) for the different HO energy quantum numbers in the interval [0, 10]. For each HO energy value, we calculated the execution time, the total error $\delta_{(E_0)}$ and the relative error $\delta_{rel(E_0)}$. The total error is calculated by exploiting the fact that the OFPC matrix is symmetric. We know the property $5HOB \times 5HOB^T = I$ where I is the identity matrix. After the multiplying, we sum up the deviations of the product matrix from an ideal unit matrix. The total error $\delta_{(E_0)}$ should increase as the matrix dimension increases, although it should stay pretty low. The relative error $\delta_{rel(E_0)}$ is the total error divided by the matrix dimension. It shows the stability of the calculation. The calculation time (in seconds) is denoted as $T(E_0)$. To examine the scalability, we used the strong scaling evaluation, where the problem size stays fixed and the number of processors is increased. Then the scaling efficiency can be measured

as the percentage of the ideal linear scaling. It can be calculated using the formula

$$Eff = \frac{t_1}{(N * t_N)} * 100\%, \tag{3.60}$$

where t_1 is the amount of the time to calculate the matrix on a single processor, N is the number of processors and t_N is the calculation time for the N processors. The efficiency calculations for P_{78} and P_{35} are presented in (fig.3.5). By increasing the number of nodes, we achieve Eff equal to 70 % on 1 node (12 processors) and it stays relatively the same for three nodes. The calculation time is plotted in (fig.3.5) using a $Log_{10} - Log_6$ scale. It is compared to the ideal parallelization, which is calculated by dividing the execution time on one processor by the number of processors. The calculations parallelized up to the three nodes show that the implementation using ScaLAPACK has good scalability (fig.3.5). The calculation time for operator P_{78} decreased from 140166 seconds on 1 processor to 5633 on 36 processors. The results for the operator P_{35} are similar. For the demonstration purposes of the 5HOBs the operators P_{78} (tbl.3.4) and P_{35} (tbl.3.5) have been calculated using the 5HOB technique. The results show that while the matrix dimensions grow significantly, the relative error stays minimal.

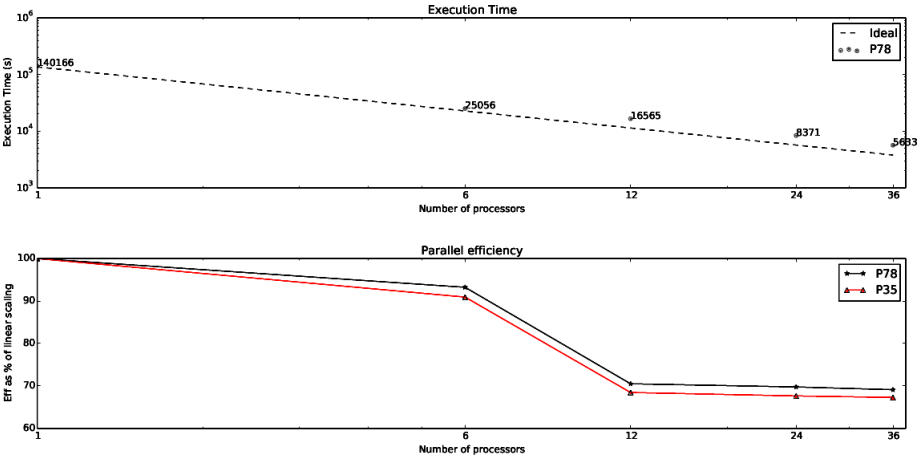


Figure 3.5: The upper graph shows the execution time in a Log_{10}/Log_6 plot, where the x-axis shows the number of processes, and on the y-axis shows the execution time in seconds. The ideal time is calculated as t_1/N where t_1 is calculation time with one node and N is the number of processes. The strong scaling efficiency as % of linear scaling for the operator P_{78} is displayed in the lower graph. Eff stands for efficiency. The number of processes is scaled in the Log_6 base. The calculations were performed with the supercomputer "HPC Sauletekis" using 3 nodes (36 cores). We used standard double precision for the calculation and the library "ScaLAPACK" for parallelism.

Table 3.4: Calculation of P_{78} using 5HOB. E means HO energy quanta; Dim is the dimension of the calculated transformation matrix; The calculation time $T(E_0)$ is presented in seconds;$\delta_{(E_0)}$ is the error of the calculation and $\delta_{rel(E_0)}$ is the relative error. The calculations were performed with the supercomputer "HPC Sauletekis", using 3 nodes (36 cores). We used standard double precision for the calculation and the library "ScaLAPACK" for parallelism.

E	Dim	$T(E_0)$	$\delta_{(E_0)}$	$\delta_{rel(E_0)}$
0	1	0.005	0	0
1	4	0.03	1.4×10^{-12}	3.6×10^{-13}
2	26	0.05	1.1×10^{-11}	4.4×10^{-13}
3	84	0.023	4.9×10^{-11}	5.9×10^{-13}
4	295	0.038	2.4×10^{-10}	8.2×10^{-13}
5	776	0.08	9.1×10^{-10}	1.2×10^{-12}
6	2044	0.79	3.6×10^{-9}	1.8×10^{-12}
7	4616	9.1	1.1×10^{-8}	2.5×10^{-12}
8	10234	94	3.6×10^{-8}	3.5×10^{-12}
9	20640	724	1.0×10^{-7}	5.0×10^{-12}
10	40712	5633	2.8×10^{-7}	6.8×10^{-12}

Table 3.5: Calculation of P_{35} using 5HOB. E means HO energy quanta; Dim is the dimension of the calculated transformation matrix; The calculation time $T(E_0)$ is presented in seconds;$\delta_{(E_0)}$ is the error of the calculation and $\delta_{rel(E_0)}$ is the relative error. Calculations were performed with the supercomputer "HPC Sauletekis", using 3 nodes (36 cores). We used standard double precision for the calculation and the library "ScaLAPACK" for parallelism.

E	Dim	$T(E_0)$	$\delta_{(E_0)}$	$\delta_{rel(E_0)}$
0	1	0.003	0	0
1	4	0.01	1.3×10^{-12}	3.2×10^{-13}
2	26	0.02	1.1×10^{-11}	4.3×10^{-13}
3	84	0.03	4.2×10^{-11}	5.0×10^{-13}
4	295	0.04	1.9×10^{-10}	6.5×10^{-13}
5	776	0.09	6.1×10^{-10}	7.9×10^{-13}
6	2044	0.8	2.2×10^{-9}	1.0×10^{-12}
7	4616	9.2	6.6×10^{-8}	1.4×10^{-12}
8	10234	89	2.0×10^{-8}	1.9×10^{-12}
9	20640	810	5.5×10^{-7}	2.6×10^{-12}
10	40712	6433	1.4×10^{-7}	3.5×10^{-12}

Summary and Conclusions

In this thesis, we present the ab-initio algebraic approach for nuclear structure calculations. To calculate the observables of the nucleus, one must ensure that the state vectors are antisymmetric and translationally invariant. These two requirements create tremendous difficulties. The antisymmetrization can be easily done using one particle coordinates, but then one is left with the problem of translational invariance. The alternative approach would be to remove the center of mass coordinate first and then antisymmetrize the state vectors. For this approach, the intrinsic Jacobi coordinates are very useful. They allow the explicit removal of said coordinate. In the nuclear physics community, the Jacobi coordinates are typically used when one has to deal with few body systems. The antisymmetrization, while not trivial, can be manageable. The few body systems do not have a large symmetric group algebra, therefore it is relatively easy to get the antisymmetric state vectors.

However, for larger systems, this approach has not been explored very deeply. As the symmetric group algebra grows, things get complicated and one has to explore the symmetric group for a way to do things efficiently. For this task, the six nucleon system is complex enough to explore. We characterize this system using the binary cluster approach with the Jacobi coordinates in the harmonic oscillator basis. We construct the coefficients of fractional parentage for three-particle subclusters and produce the state vectors for the whole system. These coefficients are constructed using the Λ operator framework. We show that only one permutation operator from the symmetric group S_6 is sufficient to achieve antisymmetrization. As this procedure is done using the intrinsic Jacobi coordinates we show that they are perfectly applicable for

p-shell nuclei. This is discussed extensively in chapter two.

We employ this framework in the coupled-J scheme. The J scheme allows reducing the model space significanly. The downside of this scheme is a meticulous work with a large amount of angular momentum recoupling coefficients. Moreover, the complicated higher-order harmonic oscillator brackets are needed to calculate the permutation operator in the angular momentum space. To tackle these difficulties, we create a systematic approach for the recoupling coefficients that make the derivation of required expressions relatively comfortable.

Another problem is the lack of generic computational tools for convenient coefficient calculation. The higher-order Talmi-Moshinsky brackets are explored in the third chapter. They allow computing the permutation operators in the Jacobi coordinate basis when more than three-particles are involved. The computational approaches are also discussed in this chapter and we show that these coefficients can be calculated efficiently on high-performance computer systems.

This makes an algebraic approach appealing for larger systems and a valuable tool for the nuclear physics community.

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Santrauka

Įvadas

Teoriniai atomo branduolio tyrimai pasižymi išskirtine modelių, skirtų jam aprašyti, gausa. Sparčios aukšto našumo kompiuterinės sistemos leido sukurti nemažai skaičiuojamosios fizikos metodų skirtų būtent šiai teorinės fizikos sričiai. Pavyzdžiui, didelės sėkmės susilaukė UNEDF projektas, kuriame buvo panaudoti taikomosios kompiuterijos metodai. Anglies-12 izotopui sėkmingai aprašyti teko sukurti kompiuterinę bibilioteką, efektyviam skaičiavimų paskirstymui ant daugiau nei 100000 branduolių [1]. Pažanga matematiniuose metoduose, naudojamų atomo branduolių aprašymui, leidžia sukurti geresnius skaičiuojamuosius modelius. To pasekoje apskaičiuojami vis didesnių ir sudėtingesnių branduolinių sistemų fizikiniai parametrai. Užduotys sprendžiamos panaudojant mažiau skaičiavimo resursų, arba greičiau. Eksperimentinė fizika teikia daug informacijos apie mikropasaulį, tačiau teorija, bent jau branduolio fizikos srityje, atsilieka nuo eksperimentų. Eksperimentiniai duomenys apie tokias sistemas, kaip pentakvarkai [2, 3, 4], ar barioninio branduolio vidinės komponentės [5, 6] yra labai svarbūs ir platesniame kontekste, todėl svarbu vystyti teorinius modelius, siekiant geresnio eksperimento paaiškinimo.

Vienas iš dažnai naudojamų banginės funkcijos bazių branduolio fizikoje yra harmoninės osciliatoriaus bazė. Harmoninio osciliatoriaus bazėje dažniausiai konstruojamos viendalelinės banginės funkcijos. Taip vadinama M-schema, kai geras kvantinis skaičius yra ne pilnutinis judesio kiekis J, o jo projekcija J_z(dar žymima, kaip M) yra labai patogi banginės funkcijos antisimetrizavimo požiūriu, panaudojant Sleiterio determinantus. Tačiau fermionus charakterizuojanti banginė funkcija turi būti ne tik antisimetriška, bet ir invariantinė transliacijų požiūriu. Sleiterio determinantų pagalba antisimetrizuota banginė

funkcija nėra transliaciškai invariantinė, dėl to reikalinga papildoma procedūra masės centro koordinatės pašalinimui. Atomo branduolys iš principo neturi masės centro, kadangi, skirtingai nei atomas, neturi centrinės sąveikos potencialo ir nepriklauso nuo išorinių laukų. Centrinis potencialas gali būti konstruojamas iš dvidalelių arba tridalelių tarpnukleoninių sąveikų, tačiau tai yra dirbtinė struktūra. Neatlikus masės centro koordinatės pašalinimo, modelio erdvė yra "užteršiama" taip vadinamom melagingom būsenom (spurious states).

Pastaraisiais metais branduolio fizikos srityje yra pastebimas susidomėjimas alternatyvomis tradiciniam viendaleliam Sleiterio determinantų metodui. Pavyzdžiui, SU_3 schema [9], taip vadinamų naturaliųjų orbitalių metodas [10], hipersferinių koordinačių metodas ir t.t. Vienas iš tokių alternatyvių metodų yra taip vadinamas algebrinis metodas. Praeitame paragrafe aptartą masės centro problemą galima išspręsti pereinant nuo viendalelių prie vidinių sistemos kooordinačių. Dvidalelinės ir tridalelinės tarpnukleoninės sąveikos branduolyje priklauso tik nuo santykinių tarpnukleoninių koordinačių. Viena iš tokių galimų vidinių koordinačių sistemų yra Jakobi koordinačių sistema [11, 12]. Normuotos Jakobi koordinačių sistemos pagrindinis privalumas yra masės centro koordinatės pašalinimas, pereinant nuo viendalelinių prie Jakobi koordinačių. Tokioje koordinačių sistemoje geri kvantiniai skaičiai gali būti pasirenkami $J^\pi T($ pilnas sistemos judesio kiekis, lyginumas, izosukinys). Šias koordinates puikiai panaudojamos harmoninio osciliatoriaus bazėje, kai atskirų kvazidalelių judesio kiekio momento kvantiniai skaičiai yra surišti panaudojant judesio kiekio momento algebrą. To pasekoje yra ženkliai sumažinamos matricų dimensijos [13]. Taip pat Jakobi koordinatės yra gan dažnai naudojamos kelių kūnų sistemų aprašymui (kai $N\leq 4$) taip vadinamame Bešerdžiame sluoksnių modelyje (No Core Shell Model (NCSM))) [14]. Sudėtingesnėms sistemoms Jakobi koordinatės naudojamos kartu su Sleiterio determinantais [14]. Posistemių antisimetrizacijai panaudojami Sleiterio determinantai, tuomet antisimetrizuoti nukleonų klasteriai yra aprašomi Jakobi koordinatėmis.

Kitas populiarus metodas yra taip vadinamas hipersferinių harmonikų metodas. Prie hipersferinių koordinačių pereinama, nuo Jakobi koordinačių. Šiame modelyje reikia skaičiuoti taip vadinamuosius Raynal-Revai ir T koeficientus [15]. Norint išvengti šių koeficiento skaičiavimo bazės konstrukcijai galima panaudoti taip vadinamas tarpinius ortogonalius pogrupius $O_{3N-3} \supset O_3 \otimes S_N$ arba $O_{3N-3} \supset O_3 \otimes O_{N-1} \supset O_3 \otimes S_N$. Tačiau ši procedūra reikalauja pakankamai sudėtingo reikalingų atvaizdų matricų skaičiavimo. Todėl

būtų naudinga turėti tokį modelį, kuris panaudotų vidines koordinates harmoninio osciliatoriaus bazėje. Toks modelis būtų lengvai įgyvendinamas skaičiavimams moderniose daugiaprocesorinėse sistemose (kompiuterių klasteriuose ar superkompiuteriuose), bei nereikalautų sudėtingų transformacijų skaičiavimų. Harmoninio oscilliatoriaus funkcijos yra labai patogios, nes viendalelinių funkcijų perstatymai sužadina ortogonalias transformacijas Jakobi koordinačių rinkiniuose. Todėl harmoninio osciliatoriaus bazėje tokių transformacių atvaizdai gali būti baigtiniai. Esminis darbo su Jakobi koordinatėmis įrankiai yra Talmi-Mošinskio transformacija [16, 17] ir harmoninio osciliatoriaus transformacijų skliausteliai (brackets) HOB. Šie skliausteliai dar žinomi kaip Talmi-Mošinskio (TMB), ar Talmi-Mošinskio-Smirnovo skliausteliai [18]. Viendaleliniai perstatymai didesnėms nei keli kūnai sistemoms lemia, kad transformuojamų Jakobi koordinačių kiekis gali augti. Todėl tampa reikalingos aukštesnės eilės Talmi-Mošinskio skliaustelių konstrukcijos [19, 20]. Sistemingas šios problemos sprendimas leistų nuosekliai konstruoti būsenos vektorius įvairioms sistemoms ar sistemoms sudarytoms iš įvairių klasterizacijų.

Yra įvairių metodikų kaip aprašyti atomo branduolio sistemą. Vienas iš jų- taip vadinamas dvinaris klasterių modelis [21]. Šiame modelyje N identiškų dalelių (Traktuojant protoną ir neutroną kaip tapatingas daleles, t.y., tos pačios dalelės dvi skirtingas būsenas) padalinama į dvi posistemes sudarytas iš N_1 ir $\mathrm{N}_2 = N - N_1$ dalelių. Jei posistemės yra antisimetrizuotos, tuomet dvidaleliniai simetrinės grupės S_N perstatymo operatoriai gali būti panaudoti visos sistemos antisimetrizacijai [22]. Tokiu būdu, yra sukonstruojami būsenos vektoriai kilminių koeficientų formalizme. Bendram atvejui galima pasirinkti, pavyzdžiui, operatorių P_{1N_1+1}. Šis operatorius sukeičia pirmą ir $N_1 + 1$ daleles vietomis. Jo poveikis transformuoja Jakobi koordinates ir transformuotų koordinačių skaičius priklauso nuo sistemos sudalijimo, bei pradinės sistemos antisimetrizacijos.

Pagrindinis tyrimo tikslas ir uždaviniai

Pagrindinis šio tyrimo tikslas yra ištirti algebrinį šešių nukleonų sistemos modelį, panaudojant Jakobi koordinates. Šiam tikslui pasiekti buvo iškelti šie uždaviniai:

- Sukurti algebrinį šešių kūnų modelį šešių nukleonų sistemoms transliaciškai invariantinėje bazėje, kai sistema yra sudaryta iš dviejų tridalelių posistemių.

– Suformuluoti sistemišką metodiką darbui su Jakobi koordinačių transformacijomis ir jų atvaizdais harmoninio osciliatoriaus funkcijų bazėje.
– Sukurti efektyvų skaitmeninį metodą šešių kūnų sistemų būsenų vektorių apskaičiavimui.
– Sukurti kompiuterinius metodus antisimetrinių būsenų vektorių skaičiavimui transliaciškai invariantinėje harmoninio osciliatoriaus bazėje.

Rezultatų naujumas ir aktualumas

Bešerdžiai ab-initio sluoksnių modelio metodai yra sėkmingai panaudojami didesnėms nei keli kūnai sistemoms. Ab-initio tipo skaitmeniniai modeliai tampa našūs, nes superkompiuterių galia nuolat auga. Teorinės fizikos vystymas, leidžiantis skaitmeniškai modeliuoti vis sudėtingesnes sistemas, yra kaip niekad aktualus siekiant tikslesnių rezultatų. Jakobi koordinatės, aprašant s- sluoksnio branduolius, yra populiarus metodas [23] dėl masės centro koordinatės eliminavimo, pereinant nuo viendalelių prie Jakobi koordinačių. Tačiau p- sluoksnio branduoliams (pvz. Litis-6) dažniau yra naudojama M-schema, arba sluoksnių modelis su šerdimi. Šešių kūnų sistema yra pakankamai didelė, kad tridalelinė nukleonų sąveika turėtų įtakos rezultatams. Taip pat tokios sistemos pagrindu galima atlikti tyrimą siekiant sukurti teorinį modelį, pritaikomą bendru atveju. Priešingai nei mažesnėse sistemose, neatsiranda įvairių supaprastėjimų. Neseniai pasirodė darbai [23], aprašantys p- sluoksnio branduolius pasinaudojant Jakobi koordinatėmis, naudoja taip vadinamą kanoninį antisimetrinių būsenų konstravimą. Šiame darbe kilminių koeficientų konstravimo problema, yra traktuojama kitaip. Pasinaudojant simetrinės grupės algebra, bei dvinarių klasterių metodika antisimetriniai būsenos vektoriai yra gaunami panaudojant taip vadinamus Λ operatorius. Šie operatoriai yra konstruojami iš atitinkamos simetrinės grupės dvidalelinių perstatymo operatorių. Matematinės fizikos požiuriu tai yra labai elegantiškas metodas, leidžiantis sistemiškai spręsti būsenų vektorių konstravimo problemą. Antisimetrizacijos procedūra yra smarkiai supaprastinama panaudojant branduolinės sistemos simetrijos sąvybes ir izosukinio formalizmą. Naudojant Jakobi koordinates sudėtingoms branduolinėms sistemoms tampa reikalingos aukštesnės eilės koordinačių transformacijos. Tokių transformacijų atvaizdai harmoninio osciliatoriaus funkcijų bazėje yra sudėtingi. Dėl to yra

tikslinga išplėtoti sistemišką ir skaitmeniškai efektyvią metodiką darbui šio modelio rėmuose. Taip pat sukurti kompiuterines programas, leidžiančias konstruoti reikalingų transformacijų atvaizdus.

Ginamieji teiginiai

1. Jakobi koordinatės yra pritaikomos antisimetrinių būsenos vektorių konstravimui šešių nukleonų sistemoms harmoninio osciliatoriaus funkcijų atvaizdavime.

2. Kilminiai koeficientai šešių nukleonų sistemai gali būti suskaičiuojami panaudojus vieną perstatymo operatorių iš simetrinės grupės S_6 generuojančio rinkinio.

3. Ab-initio algebrinis metodas leidžia sukonstruoti modelinę erdvę racionaliai panaudojant kompiuterinius resursus.

4. Būsenų vektorių konstravimas transliaciškai invariantinėje bazėje gali būti atliktas sistemiškai, to pasekoje metodas tinkamas sudėtingoms branduolinėms sistemoms aprašyti.

Autoriaus indėlis ir rezultatų aprobacija

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3. OpenReadings 2015, Vilnius: "Efficient 9j symbol and harmonic oscillator transformation brackets evaluation for binary cluster calculation"(A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

4. OpenReadings 2016, Vilnius: "Calculation of five particle harmonic-oscillator transformation brackets in translational invariant basis"(A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

5. „28th Indian-Summer School of Physics, Ab Initio Methods in Nuclear Physics" Prague, Czech Republic, 2016: „Calculation of five particle harmonic-oscillator transformation brackets in translational invariant basis"(A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

6. OpenReadings 2017, Vilnius: "Construction of antisymmetric basis states for six body systems in translationally invariant basis"(A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

7. LNFK-42, 2017: "Kilminių koeficientų skaičiavimas šešių kūnų sistemoms naudojant transliaciškai invariantinė bazė"(A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

8. "Advances in Theoretical Nuclear Physics: Probing fundamental interactions by low energy excitations", Stockholm Sweden, 2017: "Antisymmetric basis states construction for six body systems in

translationally invariant basis“(A.Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

9. OpenReadings 2018, Vilnius: “Different types of Clusterization of six body systems using Jacobi coordinates“(A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

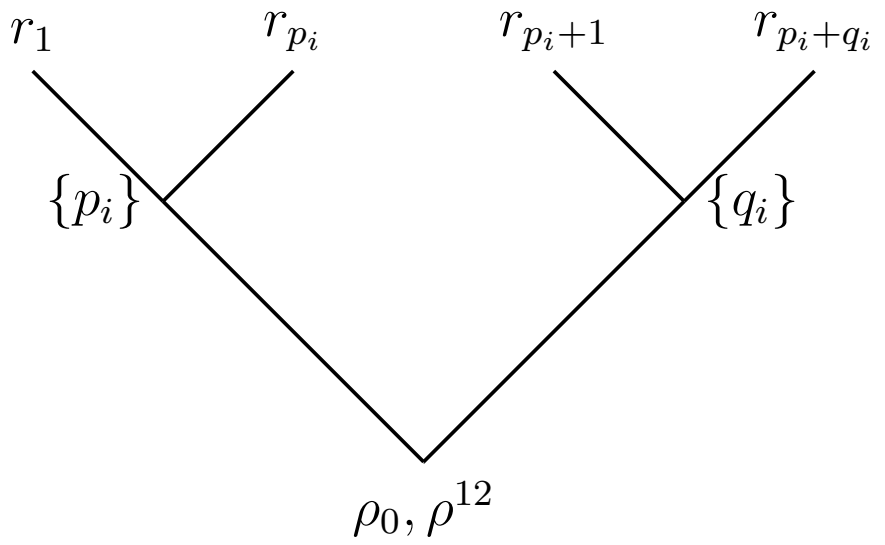
10. LNFK-43, Kaunas: “Šešių kūnų sistemos transliaciškai invariantinėje bazėje“(A. Stepšys, S. Mickevičius, D. Germanas, R.K. Kalinauskas)

Jakobi koordinatės

Atomo branduolys yra kvantinė sistema, kuri yra invariantiška transliacijų erdvėje atžvilgiu. Nukleonai, protonai ir neutronai, sudarantys atomo branduolį, tarpusavyje sąveikauja ne centriniame lauke, o dvidalelinėmis, tridalelinėmis tarpusavio sąveikomis. Taigi, sąveikos stiprumas priklauso nuo atstumo tarp sąveikaujančiu nukleonų. Naudojant įprastas koordinates yra gaunamos būsenos, kurios priklauso ne tik nuo atstumų tarp nukleonų, bet ir nuo masės centro koordinatės. Kadangi sistemos potencialas nuo masės centro koordinatės nepriklauso, tai tokios būsenos bus nefizikinės. JOs yra vadinamos melagingomis būsenomis (spurious states). Vienas iš būdų išspręsti šia problemą yra pereiti nuo viendalelių koordinačių prie vidinių sistemos koordinačių. Tokia koordinačių sistema yra normalizuotosios Jakobi koordinatės. Ši koordinačių sistema išreiškiama kaip spinduliai- vektoriai tarp dalelių ir dalelių grupių masės centrų. Ortogonalios transformacijos pagalba pereinant nuo viendalelių prie Jakobi koordinačių proporcinga masės centrui koordinatė yra atskiriama nuo kitų ir tampa invariantiška kitų koordinačių perstatymams, taigi, atskiriama. Dėl to toliau galima dirbti ne su $3N$ koordinačių, o su $3(N-1)$ [24].

Jakobi koordinatės yra konstruojamos pagal pasirinktą Jakobi medį [25]. Jakobi medis (pav. 1) yra grafas, sudarytas iš $2N-1$ viršūnių. $\mathbf{r}_j$ yra viendalelės koordinatės, ρ_0- koordinatė proporcinga masės centro koordinatei, o ρ^{12} yra santykinio judėjimo tarp dalelių klasterių koordinatė.

Jakobi medžio kairėje esančios viršūnės yra žymimos kaip p_i, o dešinėje- q_i. Proporcingos masės centrui koordinatės išraiška yra ρ_0 :



1 pav. Jakobi medis

$$\rho_0 = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \mathbf{r}_j. \tag{1}$$

Jeigu naudojamas dvinarių klasterių metodas, tuomet viršutinis indeksas ρ žymi dalelių klasterį. Apatinis indeksas žymi koordinatės numerį klasteryje. Pavyzdžiui, pirmo klasterio antroji Jakobi koordinatė bus žymima kaip ρ_2^1.

Jakobi koordinatėse galima naudoti surištą harmonio osciliatoriaus funkcijų bazę su „gerais" kvantiniais skaičiais $J^\pi T$. Gerais kvantiniais skaičiais vadiname operatorių, komutuojančių su sistemos Hamiltonianu tikrines vertes [26]. Tokioje bazėje viendalelių koordinačių perstatymai žadina ortogonalias transformacijas Jakobi koordinatėse, o tokių transformacijų atvaizdai yra baigtiniai. Teorinėje fizikoje harmoninio osciliatoriaus funkcijos yra labai plačiai naudojamos banginių funkcijų aproksimacijai. Problematiška yra tai, kad HO banginės funkcijos asimptotika yra proporcinga $\propto e^{-\alpha r^2}$, kai, tuo tarpu, aproksimuojama banginė funkcija turėtų turėti eksponentinę asimptotiką $\propto e^{-\alpha r}$. Todėl tampa reikalingi pakankamai dideli HO sužadinimai siekiant gero konvergavimo. Taip vadinama J-schema, kur kaip geras kvantinis skaičius panaudojamas sistemos pilnutinis judesio kiekio momentas J, leidžia gerokai sumažinti matricų dimensijas.

Alternatyvi J-schemai M-schema, kur geras kvantinis skaičius yra pilnutinio judesio kiekio momento projekcija J_z, dar žymimas kaip M. Ši bazė yra labai patogi Sleiterio determinantų skaičiavimui viendalelėse koordinatėse, tačiau darbui Jakobi koordinatėse yra netinkama ir lemia labai dideles retų matricų dimensijas. Matricų dimensijas galima dar labiau sumažinti, jei judesio kiekio momentai yra surišami panaudojant judesio kiekio momento algebrą.

Harmoninio osciliatoriaus funkcijų bazė

Šiame darbe atomo branduolio banginės funkcijos aproksimacijai yra panaudoja harmoninio osciliatoriaus (HO) funkcijų bazė. Ši bazė yra patogi ir dažnai naudojama teorinėje branduolio fizikoje. Viena iš pagrindinių to priežasčių yra tai, kad HO bazėje galima sukonstruoti baigtinius atvazidus. Šis aspektas yra labai svarbus naudojant Jakobi koordinates. Viendalelių koordinačių perstatymai indukuos ortogonalias transformacijas Jakobi koordinačių bazėje. Nepaisant to, kad jų atvaizdai Hilberto erdvėje bus begaliniai, pasinaudojus HO funkcijų savybėmis galima konstruoti baigtinius atvaizdus. Išraiška, pagal kurią paskiros Jakobi koordinatės susiejamos su ortonormuota HO funkcija

$$\phi_{elm}\left(\boldsymbol{\rho}\right) = (-1)^n \left[\frac{2\left(n!\right)}{\Gamma\left(n+l+3/2\right)}\right]^{\frac{1}{2}} e^{\left(-\rho^2/2\right)} \rho^l L_n^{(l+1/2)}\left(\rho^2\right) Y_{lm}\left(\boldsymbol{\rho}/\rho\right). \tag{2}$$

HO funkcijos leidžia konstruoti būsenų vektorius $|J^\pi T\rangle$ formalizme. T.y., pilnutinį judesio kiekio momentą J, bei izosukinį T panaudoti kaip gerus kvantinius skaičius. Dirbant HO funkcijų bazėje su Jakobi koordinatėmis labai svarbi konstrukcija yra Talmi-Mošinskio transformacija ir HO skliausteliai, dar žinomi kaip Talmi-Mošinskio skliausteliai. Talmi-Mošinskio transformacija yra apibrėžiama, kaip SO_2 grupės ortogonali transformacija

$$\begin{pmatrix} \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} \\ \sqrt{\frac{1}{1+d}} & -\sqrt{\frac{d}{1+d}} \end{pmatrix}, \tag{3}$$

kuri leidžia atvaizduoti viendalelius koordinačių perstatymus Jakobi koordinačių bazėje. HO skliausteliai

$$\langle e_1 l_1, e_2 l_2 : L | e_1' l_1', e_2' l_2' : L \rangle_d \tag{4}$$

leidžia tokią SO_2 transformaciją atvaizduoti HO funkcijų bazėje. Tai yra pagrindinis įrankis, dirbant su simetrinės grupės perstatymo operatorių atvaizdais.

Redukuotinio Hamiltoniano formalizmas

Norint apskaičiuoti atomo branduolio ryšio energiją yra reikalingas Hamiltonianas. Branduolinę sistemą sudaro nukleonai, sąveikaujantys tarpusavyje stipriąja ir elektromagnetine sąveikomis. Hamiltonianą sudaro kinetinės ir potencinės energijos nariai. Kinetinės energijos narys yra paprastas, o potencinės energijos narys yra pakankamai komplikuotas. Didžiausią įtaką potencialui daro nariai, aprašantys dvidalelines sąveikas, nors esant pakankamai didelės sistemoms (pavyzdžiui, šešių nukleonų sistemose) tridalelinė sąveika taip pat pasidaro ženkli. Šiame darbe yra dirbama tik su dvidalelinėmis sąveikomis. Dirbant tik su dvidalelinėms jėgomis N nukleonų sistemos Hamiltonianas gali būti užrašytas kaip dvidalelių Hamiltonianų suma [27]

$$H = \sum_{i=1<k}^{N} h\left(i,k\right). \tag{5}$$

. Šioje išraiškoje $h\left(i,k\right)$ yra taip vadinamas redukuotinis Hamiltonianas (RH)

$$h\left(i,k\right) = -\frac{\hbar^2}{2mN}\left(\nabla_i - \nabla_k\right)^2 + V\left(r_i - r_k, \sigma_i\tau_i\sigma_k'\tau_k'\right), \tag{6}$$

kur $\hbar$ yra redukuotoji Planko konstanta, m - nukleono masė, N-nukleonų skaičius. Dvidaleliniame vaizdinyje sąveikos stipris priklauso nuo atstumo tarp nukleonų $r_i - r_k$, sukinio σ ir izosukinio τ.

Dažniausiai naudojama skaičiavimams tarpnukleoninė sąveika yra fenomenologinės kilmės, o būsenoms yra taikoma izosukinio aproksimacija. Izosukinio formalizme, protonas ir neutronas yra laikomi dviem vienos dalelės būsenomis. Toks artinys gali būti naudojamas, jeigu izosukinio simetrijos pažaida yra nedidelė. Kadangi masių skirtumas tarp protono ir neutrono yra nežymus ($1.39\ Mev/c^2$.) ir sudaro tik apie 0.147% neutrono ir 0.148% protono masių, izosukinio simetrijos pažaida yra labai maža. Taigi, izosukinio aproksimacija šioms dalelėms yra pakankamai tiksli. Redukuotinio Hamiltoniano išraiška yra perrašoma įvedant Jakobi koordinates izosukinio formalizme. Tam tikslui yra įvedama bedimensinė dviejų dalelių Jakobi

koordinatė

$$\rho = \frac{1}{\sqrt{2}b}\left(\mathbf{r} - \mathbf{r}'\right). \tag{7}$$

Tuomet RH yra perrašomas, panaudojant šią koordinatę, gaunant išraišką, vadinamą bedimensiniu Redukuotiniu Hamiltonianu [27], kuris, pridėjus ir atėmus koordinatę ρ^2 ir pergrupavus narius, pavirsta į bedimensinio HO ir skirtumo tarp HO ir tikrosios sąveikos sumą.

$$h = \frac{2}{N}\left[\frac{1}{2}\left(-\Delta_\rho + \rho^2\right)\right] + \left(\frac{1}{\hbar\omega}v\left(\sqrt{2}b\rho, \sigma\tau\sigma'\tau'\right) - \frac{1}{N}\rho^2\right). \tag{8}$$

Pasinaudojant šia išraiška galima konstruoti Redukuotinį Hamiltonianą įvairiems atomo branduoliams. Šešių kūnų sistemai jis tampa

$$H_6 = 15\hbar\omega\left(\frac{2}{6}[h_0] + \frac{V\left(\sqrt{2}b\xi_2, \sigma_2\tau_2\sigma_3\tau_3\right)}{\hbar\omega} - \frac{1}{6}\rho^2\right), \tag{9}$$

kur h_0 yra jau minėtas HO Hamiltonianas.

Naudojant izosukinio formalizmą, kažkuriuo momentu reikia "atstatyti tiesą", t.y. pradėti traktuoti protoną ir neutroną kaip dvi skirtingas daleles. RH formalizme, tai yra atliekama skaičiuojant potencinės energijos matricinius elementus. Kai izosukinys yra lygus 0, izosukinio projekcija gali įgyti tik vieną vertę. Ši būsena yra vadinama singletine. Kai izosukinys yra lygus vienetui mes turime tris galimas projekcijos vertes: -1, 0, 1. Ši būsena yra vadinama tripletine. Tarpnukleoninė sąveika yra skirtinga kiekvienoje iš šių būsenų $V_{PN}(m_t = 0)$, $V_{NN}(m_t = 1)$, $V_{PP}(m_t = -1)$. Taigi, dviejų nukleonų sąveika yra išreiškiama kaip šių trijų narių suma, su atitinkamais normalizuotais koeficientais, kurie priklauso nuo branduolio struktūros [28]

$$V^{j\pi t}\left(r_{ik}\right) = \sum_{m_t} c_{tm_t} V^{j\pi t m_t}\left(r_{ik}\right). \tag{10}$$

Pavyzdžiui, litis-6 turi tris neutronus ir tris protonus, o berilis-6 yra sudarytas iš keturių protonų ir dviejų neutronų. Atomo branduolio ryšio energija yra suskaičiuojama užpildant Hamiltoniano matricą, transformuojant ją į antisimetrinį poerdvį ir diagonalizuojant gautą matricą. Žemiausia tikrinė vertė bus ryšio energija.

Antisimetrinio poerdvio konstravimas

Norint užtikrinti Pauli draudimo principą, bangines funkcijas, arba būsenos vektorius, reikia antisimetrizuoti. Sleiterio determinantai

leidžia atlikti šią procedūrą pakankamai nesunkiai naudojant viendalelines koordinates. Tačiau, kaip jau buvo minėta, vietoj 3N viendalelinių koordinačių, užtenka panaudoti 3(N-1) koordinatę [24] atomo branduolio aprašymui. Sleiterio determinantai leidžia sukonstruoti daugiadalelinę banginę funkciją iš viendalelinių banginių funkcijų superpozicijos. Tokį pat poveikį galima formalizuoti per taip vadinamą Antisimetrizatorių. Šis operatorius yra apibrėžiamas kaip simetrinės grupės visų perstatymo operatorių suma

$$A_{1,\ldots,N} = \frac{1}{N!} \sum_{P \in S_N} \pi_P P. \tag{11}$$

Jo tikriniai vektoriai yra vadinami kilminiais koeficientais. Šie koeficientai žymi neantisimetrizuotų arba dalinai antisimetrizuotų posistemių būsenos vektorių transformaciją į antisimetrinį visos sistemos poerdvį. Matematinis Sleiterio determinantų mechanizmas gali būti paaiškintas panaudojant grupių teoriją. Galima padaryti išvadą, kad panaudojant grupių teorijos, o tiksliau simetrinės grupės savybes, galima sukurti efektyvesnę antisimetrizacijos metodiką.

Kilminiai koeficientai leidžia sistemą antisimetrizuoti palaipsniui. Vietoj visos sistemos antisimetrizacijos iš karto, panaudojant aibę perstatymo elementų, galima iš pradžių antisimetrizuoti, pavyzdžiui, dvidaleles posistemes. Turint du antisimetrizuotus dvidalelinius poerdvius, iš jų galima išskirti antisimetrišką keturdalelinį poerdvį. Tai galima atlikti kanoniškai – iš pradžių dirbat su dviem dalelėm, tada pereinant prie trijų, keturių dalelių sistemų, arba panaudoti dvinarių klasterių formalizmą. Šiame vaizdinyje sistema yra padalinama į dvi dalis, turinčias savo vidinę struktūrą. Pirma antisimetrizuojamos posistemės, o paskui iš šių dviejų antisimetriškų poerdvių sukonstruojami pilnos sistemos antisimetriški būsenos vektoriai. Tokiu atveju yra dirbama su simetrinės grupės grandinėle

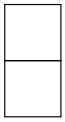
$$S_N \supset S_{N_1} \times S_{N_2}. \tag{12}$$

Šioje disertacijoje kilminiams koeficientams sukonstruoti buvo panaudotas Λ operatorius [24], kuris yra apibrėžiamas kaip simetrinės grupes S_N visų dvidalelinių operatorių suma:

$$\Lambda = \sum_{i<j=1}^{N} P_{ij}. \tag{13}$$

Kadangi visi aukštesnės eilės perstatymo operatoriai gali būti išreikšti per dvidalelinius perstatymus (pvz., $P_{123} = P_{12}P_{23}$), simetrinės grupės

dvidaleliniai perstatymo operatoriai gali būti suprantami kaip visų grupės perstatymo operatorių generuojantys elementai. Diagonalizavus tokio operatoriaus matricą, gaunamos tikrinės vertės, identifikuojančios grupės neredukuojamus įvaizdžius[1]. Kiekviena simetrinė grupė turi simetrinį ir antisimetrinį neredukuojamą įvaizdį, bei tam tikrą kiekį tarpinės simetrijos įvaizdžių. Grafinis neredukuojamų įvaizdžių vaizdavimo būdas yra taip vadinamos Jungo diagramos (pavyzdžiai pav. 2, 4, 6), dar žymimos $[\lambda] = [\lambda_1, \lambda_2, ..., \lambda_N]$ [29]. Jungo diagrama yra sujungtų kvadratinių lastelių rinkinys. Horizontaliai prijungta ląstelė simetrizuoja įvaizdį, o vertikaliai prijungta ląstelė antisimetrizuoja. Neredukuotinių poerdvių matriciniai atvaizdai yra



$$[\lambda] = [11].$$

2 pav. Jungo schema žymima [11], atitinkanti antisimetrinį dvidalelinį poerdvį.

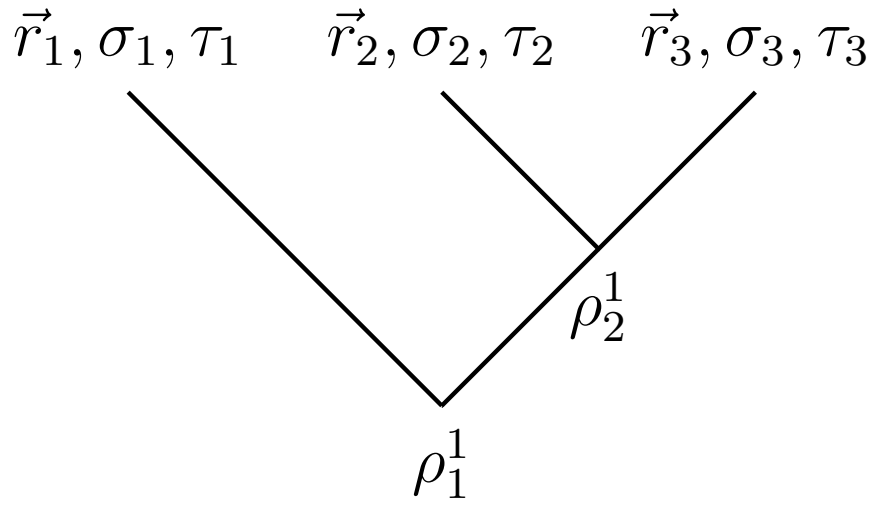
identifikuojami pagal Λ operatoriaus tikrines vertes, kuri surandama iš atitinkamo poerdvio Jungio diagramos. Kuri vertė atitinka kurį poerdvį mes randame pasinaudodami išraiška [24]

$$\Lambda(\lambda) = \frac{1}{2}\sum_{i=1}^{n}\lambda_i(\lambda_i - 2i + 1). \tag{14}$$

Šioje išraiškoje n yra Jungo diagramos eilutės numeris, o λ_i yra dėžučių kiekis kiekvienoje iš eilučių, i yra eilutės indeksas.

Λ operatorius yra sudalomas atsižvelgiant į sistemos, kuriai konstruojamas operatorius Jakobi koordinačių struktūrą. Trijų kūnų sistemą, sudarytą iš fermionų galime sudalinti į du subklasterius, sudarytus iš vienos ir dviejų dalelių ($N_1 = 1$ ir $N_2 = 2$) (pav. 3). Tokiai

[1] Neredukuojamas įvaizdis – fundamentalus grupės įvaizdis, kurį galima panaudoti atvaizduojant iš principo redukuojamus įvaizdžius.



3 pav. Jakobi medis trijų nukleonų sistemai. ρ_y^x yra Jakobi koordinatė, kur x yra klasterio numeris, y yra koordinatės numeris, r- dalelės orbitinė koordinatė, σ - sukinio koordinatė, τ - izosukinio koordinatė.

sistemai Jakobi koordinatės yra

$$\begin{aligned} \boldsymbol{\rho}_1^1 &= \sqrt{\frac{2}{3}}(\boldsymbol{r}_1 - \frac{1}{2}(\boldsymbol{r}_2 + \boldsymbol{r}_3)), \\ \boldsymbol{\rho}_2^1 &= \frac{1}{\sqrt{2}}(\boldsymbol{r}_2 - \boldsymbol{r}_3). \end{aligned} \tag{15}$$

Šiai sistemai simetrinės grupės grandinėlė būtų

$$S_3 \supset S_1 \times S_2. \tag{16}$$

S_1 grupė yra triviali. Tokiai sistemai Λ operatoriaus išraiška yra

$$\Lambda = P_{12} + P_{13} + P_{23}. \tag{17}$$

Perstatymo operatorių P_{12} ir P_{13} poveikis sistemos koordinatėms pasireikš dalelių perstatymu tarp klasterių. Tuo tarpu perstatymo operatorius P_{23} perstatys nukleonus antro klasterio viduje. Šis klasteris taip pat yra antisimetrizuojamas. Λ operatorius yra užrašomas, panaudojant dvidalelinį operatorių $\overline{\Lambda}_2\left(\left[1^2\right]\right)$, kuris priklauso nuo pilnai antisimetriško dvidalelio neredukuotinio poerdvio $\left[1^2\right]$ (pav. 2):

$$\Lambda = P_{12} + P_{13} + \overline{\Lambda}_2(\lambda_2). \tag{18}$$

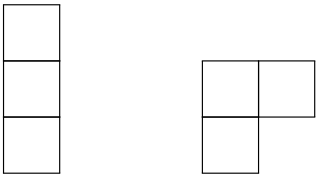
Kadangi yra dirbama su antisimetriškais sistemos poklasteriais, tai abu tarpklasteriniai perstatymo operatoriai turės tokį pat poveikį. Atsižvelgus į tai ir atlikus lygties narių pergrupavimus gauname galutinę išraišką

$$P_{13} = \frac{1}{2}(\Lambda - \overline{\Lambda}_2(\lambda_2)). \tag{19}$$

Iš šios lygties galima padaryti išvadą, kad turint antisimetrizuotus poerdvius, vieno perstatymo elemento užtenka, kad atvaizduoti anksčiau aprašytų Λ operatorių poveikį. Šis metodas veikia dvinarių klasterių formalizmui bet kokio dydžio sistemoms. Bendra tokio tipo operatorių išraiška dvinarių klasterių formalizme yra [30]

$$P_{1N_1+1} = \frac{1}{N_1 N_2}\left(\Lambda(\lambda) - \overline{\Lambda}_1\left(\left[1^{N_1}\right]\right) - \overline{\Lambda}_2\left(\left[1^{N_2}\right]\right)\right). \tag{20}$$

Λ operatoriaus poveikis gali būti apibūdintas vienu laisvai pasirenkamu dvidaleliniu operatoriumi, pavyzdžiui P_{1N_1+1}, perstatančiu daleles iš pirmo ir antro klasterių. Trijų kūnų atveju, turint antisimetrizuotą dviejų dalelių klasterį, antisimetrinė Jungo schema yra $[1^2]$. Tada trims nukleonams galimos Jungo schemos yra dvi: pilnos antisimetrijos ir dalinės antisimetrijos (pav. 4). Apibūdinti Λ operatorių mes pasirenkame operatorių P_{13}



$a)[\lambda_1] = [1^3]$ $\quad$ $b)[\lambda_2] = [21]$

4 pav. Jungo schemos, atitinkančios grupės S_3 antisimetrinį ir dalinės antisimetrijos neredukuotinius poerdvius. a) yra antisimetrinis poerdvis $[1^3]$. b) yra dalinės antisimetrijos poerdvis [21].

Operatoriaus P_{13} atvaizdas HO funkcijų bazėje yra

$$\begin{aligned}
&\langle(((e_1 l_1, \frac{1}{2})j_1, (\overline{E_1 L_1}, \overline{S}_1)\overline{J}_1); (\frac{1}{2}, \overline{T}_1)\left[1^2\right])E_1 J_1 T_1 | P_{13} \times \\
&|(((e_1' l_1', \frac{1}{2})j_1', (\overline{E}_1' \overline{L}_1', \overline{S}_1')\overline{J}_1'); (\frac{1}{2}, \overline{T}_1')\left[1^2\right])E_1 J_1 T_1\rangle \\
&= (-1)^{L+\overline{L}'+\overline{S}+\overline{S}'+\overline{T}+\overline{T}'} \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \overline{T}_1' \\ \frac{1}{2} & \overline{T}_1 & T \end{bmatrix} \qquad (21) \\
\times \sum_{LS} (-1)^L &\begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \overline{S}_1' \\ \frac{1}{2} & \overline{S}_1 & S \end{bmatrix} \begin{bmatrix} l_1 & \overline{L}_1 & L \\ \frac{1}{2} & \overline{S_1} & S \\ j_1 & \overline{J}_1 & J \end{bmatrix} \begin{bmatrix} l_1' & \overline{L}_1' & L \\ \frac{1}{2} & \overline{S}_1' & S \\ j' & \overline{J}_1' & J \end{bmatrix} \\
&\times \langle e_1 l_1, \overline{E}_1 \overline{L}_1 : L | \overline{E}_1' \overline{L}_1', e_1' l_1' : L \rangle_3 .
\end{aligned}$$

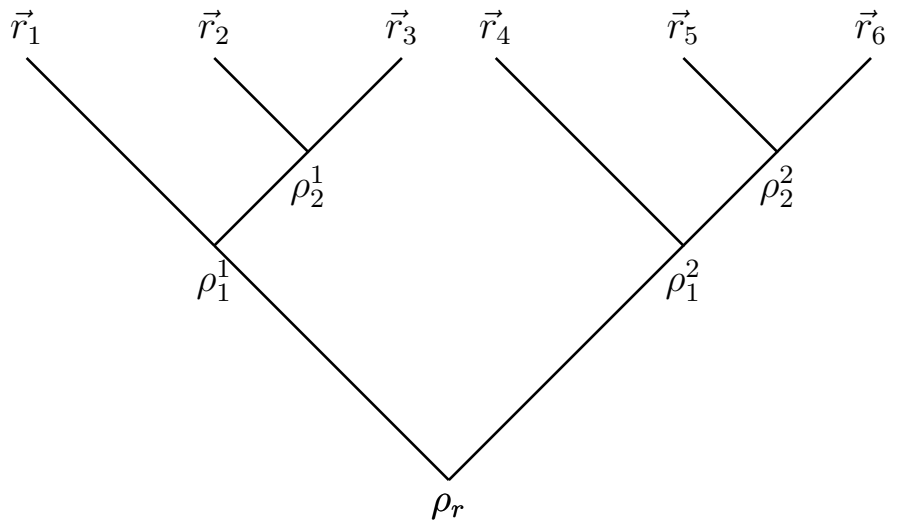
Operatoriaus poveikis yra sudarytas iš keturių judesio kiekio perrišimo koeficientų ir Talmi-Mošinskio skliaustelių. Judesio kiekio momento perrišimo koeficientai yra išreiškiami per taip vadinamus 9j simbolius, o koeficientai, kuriuose yra 0 vertė, per paprastesnius 6j simbolius. Diagonalizavus šia matricą, yra gaunami tikriniai vektoriai, kurie vadinami kilminiais koeficientais. Šie koeficientai

$$\langle(((e_1 l_1, \frac{1}{2})j_1, (\overline{EL}, \overline{S})\overline{J}); (\frac{1}{2}, \overline{T})\left[1^2\right])EJT | EJT\Delta\left[1^3\right]\rangle \qquad (22)$$

leidžia atlikti transformaciją nuo antisimetriškos dviejų nukleonų atžvilgiu bazės, prie pilnai antisimetriškos tridalelės bazės.

Šešių nukleonų antisimetrinių būsenų konstravimas

Norint gauti antisimetrinį poerdvį šešių nukleonų sistemai, reikia atlikti panašią veiksmų seką kaip ir trijų nuleonų sistemos atveju. Šiame darbe yra nagrinėjamas atvejis, kai šešių kūnų sistema yra padalinta į tridalelines posistemes (pav. 5).



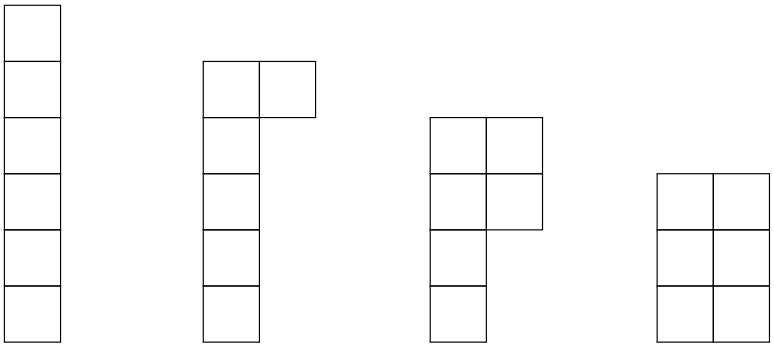
5 pav. Jakobi medis šešių nukleonų sistemai, padalintai į tridalelines posistemes.

Tokiai sistemai Jakobi koordinatės yra

$$\begin{aligned}
\rho_1^1 &= \sqrt{\frac{2}{3}}(\boldsymbol{r}_1 - \frac{1}{2}(\boldsymbol{r}_2 + \boldsymbol{r}_3)),\\
\rho_2^1 &= \frac{1}{\sqrt{2}}(\boldsymbol{r}_2 - \boldsymbol{r}_3),\\
\rho_1^2 &= \sqrt{\frac{2}{3}}(\boldsymbol{r}_4 - \frac{1}{2}(\boldsymbol{r}_5 + \boldsymbol{r}_6)),\\
\rho_2^2 &= \frac{1}{\sqrt{2}}(\boldsymbol{r}_5 - \boldsymbol{r}_6),\\
\rho_r &= \frac{1}{\sqrt{6}}(\boldsymbol{r}_1 + \boldsymbol{r}_2 + \boldsymbol{r}_3 - \boldsymbol{r}_4 - \boldsymbol{r}_5 - \boldsymbol{r}_6).
\end{aligned} \tag{23}$$

Turint antisimetrizuotas posistemes, galimas S_6 grupės neredukuotinų poerdvių rinkinys iš keturių Jungo diagramų (pav. 6).

Kaip ir ankščiau aptartu trijų nukleonų atveju, yra suskaičiuojamas dvidalelinio perstatymo operatoriaus (pvz. P_{14}) atvaizdas HO funkcijų bazėje ir jis yra diagonalizuojamas. Gauti tikriniai vektoriai yra šešių nukleonų sistemos kilminiai koeficientai, leidžiantys transformuoti būsenos vektorius iš turinčius antisimetrizuotas tridaleles posistemes į



$a)[\lambda_1] = [1^6]$ $b)[\lambda_2] = [21^4]$ $c)[\lambda_3] = [2^2 1^2]$ $d)[\lambda_4] = [2^3]$

6 pav. Keturios galimos Jungo diagramų konfiguracijos, atitinkančios šešių nukleonų sistemos neredukuotinius poerdvius antisimetrizuotoms trijų nukleonų posistemėms. a) yra pilnai antisimetrinis poerdvis $[1^6]$. Konfiguracijos b),c),d) yra žemesnės antisimetrijos.

pilnai antisimetrinį šešių nukleonų poerdvį

$$\langle(\big(E_1 J_1 T_1 \Delta_1, E_2 J_2 T_2 \Delta_2)\overline{J}, el\big)\, E_6 J_6 T_6 \left[1^3\right] \left[1^3\right] | E_6 J_6 T_6 \Delta_6 \left[1^6\right] \left[1^3\right] \left[1^3\right]\rangle. \tag{24}$$

S_6 grupės operatoriaus P_{14} atvaizdo konstravimas HO funkcijų bazėje yra gan komplikuotas. Iš pradžių yra atliekama šio operatoriaus atvaizdo faktorizacija, norint atskirti izosukininę dalį

$$\langle P_{14}\rangle = \langle P_{14}^{\sigma r}\rangle \langle P_{14}^{\tau}\rangle . \tag{25}$$

Sekantis žingsnis yra sukinio-orbitos atsiejimas

$$\langle P_{14}^{\sigma r}\rangle = \langle P_{14}^{\sigma}\rangle \langle P_{14}^{r}\rangle . \tag{26}$$

Sukininės ir izosukininės P_{14} išraiškos yra analogiškos ir išreiškiamos per vieną judesio kiekio momento perrišimo koeficientą

$$\begin{aligned}\big\langle((s_1,\overline{S}_1)S\,_1,(s_2,\overline{S}_2)S\,_2)S_{12}\big|\, P_{14}^{\sigma}\,\big|((s_1',\overline{S}_1)S'\,_1,(s_2',\overline{S}_2)S'\,_2)S_{12}\big\rangle \\ = (-1)^{S_1+S_1'}\begin{bmatrix} \overline{S}_1 & \frac{1}{2} & S_1' \\ \frac{1}{2} & \overline{S}_2 & S_2' \\ S_1 & S_2 & S_{12}\end{bmatrix}.\end{aligned} \tag{27}$$

Daug problematiškesnis yra L-S ryšio atsiejimas ir orbitinė dalis. L-S ryšio atsiejimo procedūros išraiška

$$\left\langle (l_r,((((l_1,s_1)j_1,(\overline{L}_1,\overline{S}_1)\overline{J}_1)J_1,((l_2,s_2)j_2,(\overline{L}_2,\overline{S}_2)\overline{J}_2)J_2)J_{12})J\right| P_{14}^{r\sigma} \tag{28}$$

$$\times\left|(l'_r,((((l'_1,s'_1)j'_1,(\overline{L}'_1,\overline{S}'_1)\overline{J}'_1)J'_1,((l'_2,s'_2)j'_2,(\overline{L}'_2,\overline{S}'_2)\overline{J}'_2)J'_2)J'_{12})J\right\rangle$$

$$= \sum_{\substack{L_1S_1\\L_2S_2\\L_{12}S_{12}\\L}}\sum_{\substack{L'_1S'_1\\L'_2S'_2\\L'_{12}S'_{12}\\L'}} \begin{bmatrix} l_1 & s_1 & j_1\\ \overline{L}_1 & \overline{S}_1 & \overline{J}_1\\ L_1 & S_1 & J_1\end{bmatrix}\begin{bmatrix} l_2 & s_2 & j_2\\ \overline{L}_2 & \overline{S}_2 & \overline{J}_2\\ L_2 & S_2 & J_2\end{bmatrix}$$

$$\times\begin{bmatrix} L_1 & S_1 & J_1\\ L_2 & S_2 & J_2\\ L_{12} & S & J_{12}\end{bmatrix}\begin{bmatrix} L_{12} & S & J_{12}\\ l_r & 0 & l_r\\ L & S & J\end{bmatrix}$$

$$\times\left\langle((l_1,\overline{L})L_1,(l_2,\overline{L}_2)L_2)L_{12},l_r)L\,|P_{14}^r|\,((l'_1,\overline{L}')L'_1,(l'_2,\overline{L}'_2)L'_2)L'_{12},l'_r)L\right\rangle$$

$$\times\left\langle((s_1,\overline{S}_1)S\,1,(s_2,\overline{S}_2)S\,2)S\,|P_{14}^{\sigma}|\,((s'_1,\overline{S}'_1)S'\,1,(s'_2,\overline{S}'_2)S'\,2)S\right\rangle$$

$$\times\delta_{\overline{L}_1\overline{L}_2,\overline{L}'_1\overline{L}'_2};\delta_{\overline{S}_1\overline{S}_2,\overline{S}'_1\overline{S}'_2};\delta_{\overline{J}_1\overline{J}_2J,\overline{J}'_1\overline{J}'_2J'}\delta_{LS,L'S'}$$

$$\times\begin{bmatrix} L'_{12} & l'_r & L'\\ S' & 0 & S'\\ J'_{12} & l'_r & J\end{bmatrix}\begin{bmatrix} L'_1 & L'_2 & L'_{12}\\ S'_1 & S'_2 & S'\\ J'_1 & J'_2 & J'_{12}\end{bmatrix}\begin{bmatrix} l'_1 & \overline{L}'_1 & L'_1\\ s'_1 & \overline{S}'_1 & S'_1\\ j'_1 & \overline{J}'_1 & J'_1\end{bmatrix}\begin{bmatrix} l'_2 & \overline{L}'_2 & L'_2\\ s'_2 & \overline{S}'_2 & S'_2\\ j'_2 & \overline{J}'_2 & J'_2\end{bmatrix}$$

reikalauja kruopštaus darbo su judesio kiekio momento perrišimo koeficientais. Operatoriaus P_{14} poveikis į orbitinę sistemos dalį susideda iš keturių judesio kiekio momento perrišimo koeficientų, bei specialios konstrukcijos pažymėtos $\langle spec.4HOB\rangle$

$$\left\langle((l_1,\overline{L})L_1,(l_2,\overline{L}_2)L_2)L_{12},l_r)L\,|P_{14}^r|\,((l'_1,\overline{L})L'_1,(l'_2,\overline{L}_2)L'_2)L'_{12},l'_r)L\right\rangle \tag{29}$$

$$\times\delta_{\overline{L}_1\overline{L}_2,\overline{L}'_1\overline{L}'_2}\delta_{l_{12r},l'_{12r}}\delta_{\overline{L}_{12},\overline{L}'_{12}}$$

$$= \sum_{\substack{l_{12}\overline{L}_{12}\\l_{12r}}}\sum_{l'_{12}} \begin{bmatrix} l_1 & \overline{L}_1 & L_1\\ l_2 & \overline{L}_2 & L_2\\ l_{12} & \overline{L}_{12} & L_{12}\end{bmatrix}\begin{bmatrix} l_{12} & l_r & l_{12r}\\ \overline{L}_{12} & 0 & \overline{L}_{12}\\ L_{12} & l_r & L\end{bmatrix}\langle spec.4HOB\rangle$$

$$\times\begin{bmatrix} l'_{12} & \overline{L}_{12} & L'_{12}\\ l'_r & 0 & l'_r\\ l_{12r} & \overline{L}_{12} & L\end{bmatrix}\begin{bmatrix} l'_1 & l'_2 & l'_{12}\\ \overline{L}_1 & \overline{L}_2 & \overline{L}_{12}\\ L'_1 & L'_2 & L'_{12}\end{bmatrix}.$$

Ši konstrukcija žymi orbitinės dalies viendalelių koordinačių perstatymo atvaizdą HO bazėje, kai yra veikiamos trys Jakobi koordinatės. Ši transformacija yra žymima

$$\left\langle (e_1 l_1, e_2 l_2)\, l_{12}, e_r l_r : l_{12r} \right| \left(e_1' l_1', e_2' l_2'\right) l_{12}', e_r' l_r' : l_{12r\ d_1 d_2}' \Big\rangle\, \delta_{l_{12r}, l_{12r}}. \quad (30)$$

Jakobi koordinačių bazėje ji apibrėžiama kaip trys dvimatės Talmi-Mošinskio transformacijos

$$T_{12}(d_1) T_{23}(d_2) T_{12}(d_1) = \quad (31)$$
$$\begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{\frac{d_2}{1+d_2}} & \sqrt{\frac{1}{1+d_2}} \\ 0 & \sqrt{\frac{1}{1+d_2}} & -\sqrt{\frac{d_2}{1+d_2}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{d_1}{1+d_1}} & \sqrt{\frac{1}{1+d_1}} & 0 \\ \sqrt{\frac{1}{1+d_1}} & -\sqrt{\frac{d_1}{1+d_1}} & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

kurių atvaizdas HO funkcijų bazėje susideda iš dviejų judesio kiekio momento perrišimo koeficientų ir trijų HO skliaustelių

$$\langle ((e_1 l_1, e_2 l_2) l_{12}, e_3 l_3) l | T_{12}(d_1) T_{23}(d_2) T_{12}(d_1) | ((e_1' l_1', e_2' l_2') l_{12}', e_3' l_3') l \rangle_{d_1 d_2} = \quad (32)$$
$$\sum_{\substack{\varepsilon_1 \lambda_1, \varepsilon_2 \lambda_2, \Lambda_{23} \\ \varepsilon_2' \lambda_2'}} \langle e_1 l_1, e_2 l_2 : L_{12} | \varepsilon_1 \lambda_1, \varepsilon_2 \lambda_2 : L_{12} \rangle_{d_1} \delta_{L_{12} e_3 l_3, L_{12}' e_3' l_3'}$$
$$\times \begin{bmatrix} \lambda_1 & 0 & \lambda_1 \\ \lambda_2 & l_3 & \Lambda_{23} \\ L_{12} & l_3 & L \end{bmatrix} \left\langle \varepsilon_2 \lambda_2, e_3 l_3 : \Lambda_{23} | \varepsilon_2' \lambda_2', e_3' l_3' : \Lambda_{23} \right\rangle_{d_2}$$
$$\times \begin{bmatrix} \lambda_1 & \lambda_2' & L_{12}' \\ 0 & l_3' & l_3' \\ \lambda_1 & \Lambda_{23} & L \end{bmatrix} \langle \varepsilon_1 \lambda_1, \varepsilon_2' \lambda_2' : L_{12} | e_1' l_1', e_2' l_2' : L_{12}' \rangle_{d_1} \delta_{L_{12}, L_{12}'}.$$

Šioms ir sudėtingesnėms struktūroms, bei jų skaičiavimo technikai, yra paskirta trečia disertacijos dalis. Šio darbo eigoje buvo atlikti skaičiavimai panaudojant superkompiuterį "HPC Saulėtekis" [31]. Panaudojant 3 mazgus buvo suskaičiuoti kilminiai koeficientai skirtingų šešių kūnų sistemų pagrindinėms būsenoms (lent. 1). Būsenai $J = 2$ ir $T = 2$ (atitinka ${}^{6}_{1}\mathrm{H}$) antisimetrinės būsenos atsiranda tik prie HO energijos sužadinimo lygaus 3. Šiuo atveju diagonalizuojamos matricos dimensija yra 212, o antisimetrinių būsenų kiekis yra 4. Būsenai $J = 0$ ir $T = 1$ (atitinka ${}^{6}_{2}$ ir ${}^{6}_{4}\mathrm{Be}$ pagrindines būsenas) pirmos dvi antisimetrinės būsenos pasirodo, kai HO energija yra lygi 2. Taip pat

yra ir ${}^{6}_{3}$Li izotopui, kurio pagrindinė būsena yra $J = 1$, $T = 0$. Gauti rezultatai rodo, kad diagonalizuotos operatoriaus P_{14} matricos tikrinės vertės atitinka numatytas.

1 lent. Tikrinių verčių atitinkančių neredukuotinius šešių nukleonų sistemos poerdvius skaičiavimas. E yra HO energijos kvantas; J-pilnutinis judesio kiekio momentas; T yra izosukinys; Dim yra P_{14} matricos dimensija; Skaičiai yra tikrinės vertės. J=0 and T=1 atitinka ${}^{6}_{2}$He, ${}^{6}_{4}$Be izotopų žemiausią sluoksnį; J=1, T=0 atitinka ${}^{3}_{3}$Li; J=2,T=2-${}^{5}_{1}$H. Skaičiavimai atlikti superkompiuteriu "HPC Sauletekis" [31], panaudojant 3 mazgus (36 procesorius). Skaičiavimuose panaudota bibliotekos "ScaLAPACK" ir "PeTSc".

E	J	T	Dim	-1	$-\frac{1}{3}$	$\frac{1}{9}$	$\frac{1}{3}$
0	1	0	1	0	0	1	0
1	1	0	10	0	2	5	3
2	1	0	63	3	12	33	15
3	1	0	282	11	63	132	76
4	1	0	1007	45	231	476	255
5	1	0	2035	86	472	947	530
6	1	0	8285	387	1988	3807	2103
1	2	2	2	0	0	1	1
2	2	2	33	0	5	16	12
3	2	2	212	4	40	101	67
4	2	2	925	24	193	436	272
5	2	2	3202	103	704	1493	902
6	2	2	9457	346	2150	4373	2588
0	0	1	1	0	0	1	0
1	0	1	7	0	1	4	2
2	0	1	44	2	8	24	10
3	0	1	192	7	41	93	51
4	0	1	679	29	151	326	173
5	0	1	2035	86	472	947	530
6	0	1	5434	244	1281	2518	1391

Išvados ir apibendrinimas

Šiame darbe buvo pristatytas algebrinis transliaciškai invariantinis metodas kilminių koeficientų radimui. Algebrinis modelis leidžia lengvai pašalinti masės centro judėjimo koordinatę pereinant prie vidinių sistemos koordinačių. Ši metodika nėra gerai ištirta sistemoms didesnėms, nei keli kūnai. Disertacijoje buvo panaudota dvinarių klasterių metodika aprašyti surištai sistemai, sudarytai iš šešių nukleonų. Darbe panaudotos Jakobi koordinatės harmoninio osciliatoriaus funkcijų bazėje, sukonstruoti kilminiai koeficientai trijų kūnų posistemėms ir visai šešių nukleonų sistemai. Kilminiai koeficientai sukonstruoti panaudojant generuojančius simetrinės grupės S_6 perstatymo operatorių rinkinius. Augant simetrinės grupės algebrai, uždavinys tampa komplikuotas todėl yra patogu išnaudoti simetrinės grupės sąvybes. Gaunama antisimetrinė modelinė erdvė yra pakankamai nedidelė šešių nukleonų sistemų fizikinių parametrų skaičiavimui ir toks modelis yra tinkamas p-sluoksnio nukleonų antisimetriniams būsenų vektoriaus gauti. Kita išspręsta problema yra bendrų skaičiavimo įrankių trūkumas tokio tipo modelių konstravimui.

Aukštesnės eilės Harmoninio osciliatoriaus skliausteliams skirtas trečias disertacijos skyrius. Šie skliausteliai yra naudingi, kai yra norima sukonstruoti perstatymo operatorių atvaizdus HO bazėje, kai yra veikiamos keturios ir penkios Jakobi kooordinatės. Taip pat darbe aptariama skaičiavimo technika, norint tokias konstrukcijas panaudoti skaičiavimams ant superkompiuterių. Tai daro algebrinį branduolio modelį naudingu branduolio fizikų bendruomenės įrankiu siekiant tirti p-sluoksnio branduolines sistemas.

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