SRG-Induced Four-Body Forces in Ab Initio Nuclear Structure

Master-Thesis von Stefan Schulz
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Vorgelegte Master-Thesis von Stefan Schulz

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Darmstadt, den 20. November 2013

(Stefan Schulz)

List of Abbreviations

3N	three-nucleon
χEFT	chiral effective field theory
χPT	chiral perturbation theory
CGC	Clebsch-Gordan coefficient
EFT	effective field theory
GFMC	Green's function monte carlo
HO	harmonic oscillator
HOB	harmonic-oscillator bracket
IT-NCSM	importance-truncated no-core shell model
LEC	low-energy constant
LO	leading order (of chiral effective field theory)
NCSM	no-core shell model
NLO	next-to-leading order (of chiral effective field theory)
N^{2}LO	next-to-next-to-leading order (of chiral effective field theory)
N^{3}LO	next-to-next-to-next-to-leading order (of chiral effective field theory)
NN	nucleon-nucleon
NO	normal ordering
QCD	quantum chromodynamics
SRG	similarity renormalization group

Contents

1 Introduction

In recent years ab initio nuclear structure calculations have become applicable to an increasing number of nuclei. Today one can calculate nuclei up to the p-shell using Green's function Monte Carlo (GFMC) [1], the no-core shell model (NCSM) [2, 3] or lattice effective field theory [4]. Lower sd-shell nuclei can be calculated with the importance-truncated no-core shell model (IT-NCSM) [5]. Even medium-mass nuclei are accessible using coupled-cluster methods [6] or the in-medium similarity renormalization group [7]. These improvements are based on increasing computational power and various improvements to reduce the computational burden.

One of the main problems in nuclear-structure calculations are the short-range correlations induced by high-precision nuclear interactions. The interaction we use is derived within chiral effective field theory (χEFT). This framework allows a systematic construction of nuclear interactions by assuming nucleons and pions to be the relevant degrees of freedom. It is restricted to the low-energy regime, as for the description of medium- and high-energy effects, e.g., nucleonic excitations, the fundamental degrees of freedom, quarks and gluons, are necessary. A connection to the underlying theory, quantum chromodynamics (QCD), is established through chiral symmetry.

The χEFT potentials also generate short-range correlations. Using Slater determinants of single-particle eigenstates of the harmonic-oscillator (HO) Hamiltonian, or any other basis that cannot represent these correlations in an appropriate manner, a large set of basis states is needed to reproduce them. Interactions that are represented in such a basis have a strong coupling between energetically low- and high-lying basis states. Thus the model space needs to include high-lying basis states for the description of low-energy nuclear states. To avoid this computationally expensive approach, one tries to reduce the coupling, using methods like the unitary correlation operator method (UCOM) [8] or the similarity renormalization group (SRG) [9]. Both greatly improve convergence for subsequent calculations [10]. We will focus on the latter in combination with the quasi-exact (IT-)NCSM. However, the methods devised in this thesis can be used in combination with non-exact calculations that are applicable to medium-mass nuclei in future work.

The SRG defines a continuous unitary transformation for operators, e.g., the Hamiltonian, by using a flow equation that can be evolved to any value of the flow parameter α. Due to the unitarity of the transformation the eigenvalues of any operator should be independent of α. Furthermore, the evolution depends on an anti-hermitian generator, which can be chosen freely and, therefore, offers great flexibility to tailor the evolution for a specific problem. A standard choice exist, which we use to drive the Hamiltonian to a band-diagonal structure in momentum space, thus reducing the coupling between low- and high-lying states [10].

While being effective in reducing correlations, the SRG induces irreducible many-body contributions. Previous works established a framework to handle initial and SRG induced three-body contributions completely [11–13]. We start with the SRG evolution of the bare nucleon-nucleon (NN) and three-nucleon (3N) interactions in a fully antisymmetrized HO basis depending on Jacobi coordinates, hereafter Jacobi basis. Neglecting four- and multi-nucleon contributions, the matrix elements are then converted to the m-scheme basis, which consists of Slater determinants of single-particle HO states. This basis is convenient for a subsequent many-body calculation, e.g., in the IT-NCSM.

However, the induced four-body forces can be strong enough to influence the results and neglecting them may prevent an accurate calculation. Using initial two- and three-body forces, the ground-state energies of heavier p-shell nuclei, e.g., ^{16}O, display a notable dependence on α [14]. This reveals the presence of sizable four-body contributions. Calculations with initial two-body forces and including their induced three-body forces are independent of α, indicating initial three-body forces to be responsible for the effect.

There have already been attempts to find different SRG generators that induce less many-body contributions, but still reduce the short-range correlations sufficiently. As these attempts have not been successful yet, we will expand the existing framework to incorporate the induced four-body contributions in our calculations. One of the goals of this thesis is to enable a reliable calculation of p- and lower sd-shell nuclei including the induced four-body contributions from the SRG. The investigation will be limited to energy levels of these nuclei. The methods we devise are applicable to other observables and initial four-body forces as well, if they need to be included in the future.

The SRG induced four-body contributions will be restricted to the channels with low angular momentum for the following investigations. The restriction is based on the observation that states with low angular momentum are

usually the most important ones for low-energetic configurations. Consequently the ^{4}He ground state is a $J = 0$ state and can be described exactly with this approximation. To check the expected behavior, we perform calculations with different number of channels, starting with the ^{4}He ground-state channel ($J = 0$,$T = 0$, positive parity) and successively including other channels. The procedure allows us to analyze the importance of different four-body channels and their effect on the α dependence. Furthermore, the model space used for the SRG transformation in four-body space needs to be truncated to HO energies that are much smaller than in the three-body case. We, therefore, investigate the effect of different truncations on the results of the many-body calculation.

A straightforward way of dealing with the additional forces is by using a full (IT-)NCSM calculation with explicit four-body forces. This approach, however, requires substantial effort. The given matrix elements must be transformed to the four-body m-scheme representation and the IT-NCSM code needs to be adjusted to deal with these forces. Using four-body matrix elements the IT-NCSM calculation consumes a significant amount of time. Furthermore, the number of four-body matrix elements in m-scheme representation increases drastically with energy, leading to a truncation of the four-body forces to model spaces much smaller than the truncation of the three-body ones. Nevertheless, it provides a quasi-exact calculation other methods can be compared to.

An approximate approach is the normal-ordering (NO) procedure, reducing the four-body contributions to zero-body up to three-body ones. Currently, we do not have any results calculated with this method as it does not offer any advantages over the full transformation for benchmarking the effects of the induced four-body force. Nevertheless it should be kept in mind, as many-body methods that currently cannot handle four-body forces explicitly become accessible with this approximation, e.g., coupled-cluster methods. The normal-ordering approximation has already shown its potential in reducing three-body to two-body interactions yielding accurate results for closed shell nuclei [6]. It can be extended to multi-reference normal-ordering, which works with open shell nuclei and yields promising results improving the standard approach [15].

For quickly getting a first impression of the effects of the induced four-body forces, we use an even simpler approximation. The easiest way to include the four-body contributions is reducing them to three-body contributions by summing over the quantum numbers of the fourth particle in a single-particle representation. As this procedure can be seen as the evaluation of a partial trace, we call it the partial-trace approximation. This approach only requires a transformation from the four-body Jacobi basis to a basis that separates the fourth particle. Such an approximation is implemented easily and it can be performed faster than any of the previously discussed methods. Furthermore, no additional truncation of the model space is required and the resulting three-body force can be used with the existing three-body framework. Similar to the standard NO case, it is limited to closed-shell nuclei. While an expansion to open-shell nuclei is possible, it is not pursued in this work.

The thesis is organized in the following way: In chapter 2 we discuss the initial interactions and their construction in the framework of χEFT. The necessary mathematical basics for this work are presented in chapter 3. They include coordinate transformations of HO states and multiple ways of changing the angular momentum coupling. All relevant bases and their advantages and disadvantages are discussed in chapter 4. This chapter also includes the relevant basis transformations, as well as a detailed explanation of the partial-trace approximation. We discuss the SRG and its peculiarities regarding four-body forces in chapter 5. Chapter 6 explains the many-body method we use, the IT-NCSM, and in chapter 7 the results are discussed. We present results for the partial-trace approximation as well as for the explicit inclusion of four-body forces in the IT-NCSM, focusing on ^{16}O. Finally, chapter 8 summarizes the work and provides an outlook.

2 Chiral Effective Field Theory

The underlying theory describing the strong interaction between nucleons is QCD. Although QCD provides a fundamental description, it is difficult to employ it for the description of nuclei, because of its non-perturbative nature in the low-energy regime. However, there are on-going efforts to calculate nuclear forces using the fundamental degrees of freedom, e.g., using lattice QCD [16–18]. For any calculation including multiple nucleons, this method is not applicable. The description of nuclei, for instance, is all but impossible except for the lightest ones. Using χEFT it is possible to formulate a systematic expansion in terms of momentum and pion mass by using nucleons and pions as effective degrees of freedom instead of quarks and gluons. In this chapter we will discuss the formulation of an effective field theory, the influence of chiral symmetry and the systematic expansion known as chiral perturbation theory (χPT). Note that we use natural units for this chapter.

2.1 Effective Field Theory

An effective field theory (EFT) attempts to construct an effective theory for a specific energy scale. It is based on the assumption that the details of high-energy dynamics are irrelevant for the description of low-energy observables. In our case we do not need quark dynamics to describe nuclei: Using protons, neutrons and pions as effective degrees of freedom is sufficient.

This scheme works best if a large energy gap exists between the degrees of freedoms considered and the ones omitted, often called a separation of scales. The next relevant heavier meson is the ρ-meson with a mass $m_\rho \approx 775$ MeV [19], which already has a much larger mass than pions $m_\pi \approx 135-140$ MeV [19]. These scales are employed to define the breakdown scale, $\Lambda_\chi \approx m_\rho$, which must be larger than the energies investigated.

Using the effective degrees of freedom, an effective Lagrangian can be constructed, which fully describes the low-energy regime. All terms and interactions that are consistent with the symmetry of the underlying theory are included, the most prominent one in our case is the approximate chiral symmetry discussed in detail in the next section.

The constructed Lagrangian contains constants that control the strength of the different couplings, they are called low-energy constant (LEC). In principle, these LECs can be calculated using the fundamental theory. In the case of QCD this is not yet possible, as the calculations are computationally demanding, therefore the LECs are fitted to experimental data.

2.2 Chiral Symmetry

In a relativistic field-theory fermion fields can be divided into the so-called right-handed and left-handed parts, which transform differently when applying a Lorentz transformation. These parts are chiral counterparts, which means that applying a parity transformation changes these parts into each other, giving rise to the description using handedness and the frequently used analogy of mirror images.

A Lagrangian exhibiting chiral symmetry allows right-handed and left-handed quarks to be rotated in isospin independently, e.g., we can rotate right-handed quarks in isospin without rotating left-handed ones. This can be expressed using two transformations for left- and right-handed parts:

$$\begin{pmatrix} u_R \\ d_R \end{pmatrix} \to e^{-i\vec{\Theta}_R \frac{\vec{\tau}}{2}} \begin{pmatrix} u_R \\ d_R \end{pmatrix}, \qquad \begin{pmatrix} u_L \\ d_L \end{pmatrix} \to e^{-i\vec{\Theta}_L \frac{\vec{\tau}}{2}} \begin{pmatrix} u_L \\ d_L \end{pmatrix}, \tag{2.1}$$

where $\vec{\tau}$ are Pauli matrices, u and d are up and down quark fields, $\vec{\Theta}$ are the rotation angles and indices R and L indicate right- and left-handed parts, respectively. Note that $\vec{\Theta}_R$ and $\vec{\Theta}_L$ can be chosen independently of each other.

We will now consider the following form of the transformations:

$$\begin{pmatrix} u_R \\ d_R \\ u_L \\ d_L \end{pmatrix} \to e^{-i\vec{\Theta}_V \frac{\vec{\tau}}{2}} \begin{pmatrix} u_R \\ d_R \\ u_L \\ d_L \end{pmatrix}, \qquad \begin{pmatrix} u_R \\ d_R \\ u_L \\ d_L \end{pmatrix} \to e^{-i\gamma_5\vec{\Theta}_A \frac{\vec{\tau}}{2}} \begin{pmatrix} u_R \\ d_R \\ u_L \\ d_L \end{pmatrix}, \tag{2.2}$$

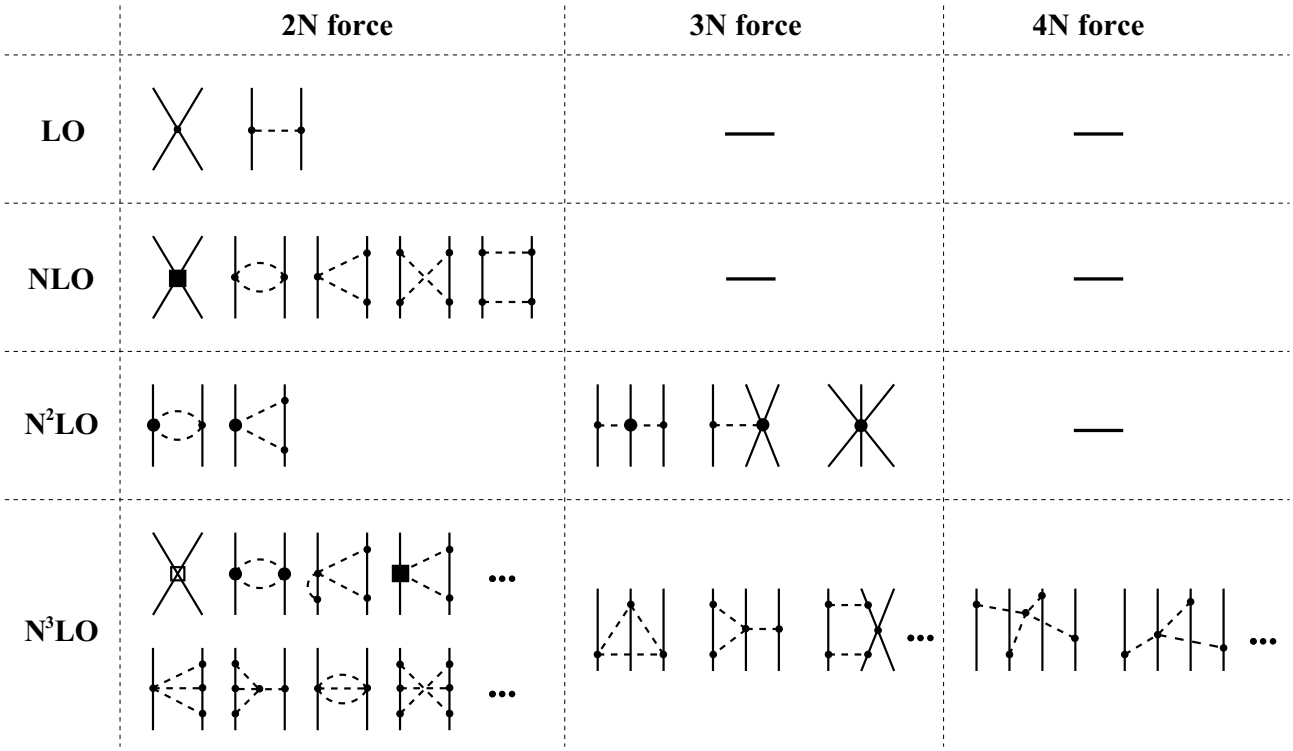


Figure 2.1: Diagrammatic depiction of χEFT interactions at different orders, where LO= $(Q/\Lambda_\chi)^0$, NLO= $(Q/\Lambda_\chi)^2$, N^{2}LO= $(Q/\Lambda_\chi)^3$ and N^{3}LO= $(Q/\Lambda_\chi)^4$. Solid and dashed lines denote nucleons and pions, respectively. Small and large dots, as well as filled and empty squares indicate different vertices.

which are called vector and axial-vector transformations as the Noether currents associated with these symmetries transform like vectors and pseudovectors, respectively [20]. The vector transformation is a rotation in isospin space for both, right- and left-handed particles and is often called isospin symmetry. The axial-vector transformation discerns between right- and left-handed particles using the operator γ_5, which yields $+1$ for right-handed fields and -1 for left-handed ones. Applying it can change a state of negative parity to a positive parity one. Note that the two descriptions of the transformations are identical and we find the following relation between the rotation angles:

$$\vec{\Theta}_V = \tfrac{1}{2}\left(\vec{\Theta}_R + \vec{\Theta}_L\right), \qquad \vec{\Theta}_A = \tfrac{1}{2}\left(\vec{\Theta}_R - \vec{\Theta}_L\right) \tag{2.3}$$

Evidence for isospin symmetry can be found easily by looking at hadronic states: All Δ-baryons have approximately the same mass, the masses of protons and neutrons are close to each other and the same is true for the masses of the three ρ mesons. All of them are examples of isospin symmetry, however, axial-vector symmetry cannot be observed. For instance the ρ-meson with a mass of 775 MeV [19] does not have a counterpart with positive parity and similar mass. The best candidate, the a_1 meson, has a mass of approximately 1230 MeV [19, 20].

One calls such a symmetry, which exists in the Lagrangian and is not realized in the ground state, spontaneously broken. Usually spontaneously broken symmetries generate massless bosons [21], also called Goldstone bosons. In our case the pions represent these bosons, however, as the symmetry is only an approximate one, they are not masseless, but they are very light compared to other mesons, which is a crucial requirement for χEFT as it entails a separation of scales.

2.3 Chiral Pertubation Theory

If we construct the Lagrangian that obeys chiral symmetry and uses pions and nucleons as effective degrees of freedom, we can use perturbative measures to derive contributions to the nuclear interaction. This is usually done using a diagrammatic approach, using solid and dashed lines for nucleons and pions, respectively. Furthermore, the different interactions between them are indicated by different kind of vertices, making it possible to construct

all contributions with these building blocks. However, an infinite number of such diagrams can be constructed and for any calculation we have to restrict ourselves to a finite number. Therefore, the diagrams are sorted by an a priori importance measure.

The usual approach is sorting them by the power of $(Q/\Lambda_\chi)^\nu$, where Q is either a nucleon momentum or the pion mass, both should be smaller than the breakdown scale Λ_χ. The power ν can be calculated from these diagrams, using Weinberg power counting [22]. Using this scheme, we find a finite number of contributions for each power of ν, which makes χEFT calculable at all. The orders are usually denoted as leading order (LO), corresponding to $\nu = 0$, next-to-leading order (NLO), which has $\nu = 2$, next-to-next-to leading order (N^{2}LO), yielding a power of $\nu = 3$ and so forth. As all contributions to $\nu = 1$ cancel, it is left out. A set of these diagrams, sorted according to their exponent ν, and the number of nucleons, is shown in Fig. 2.1.

Note that in this diagrammatic view we have vertices that indicate interactions between pions or pion-nucleon interactions or even purely nucleonic ones. These interactions are connected to the aforementioned LECs, effectively hiding all high-energy quark dynamics in a few constants. Another benefit are many-body forces that appear naturally in this framework. Three body-forces first appear in N^{2}LO and four-body ones in N^{3}LO. As higher order contributions are expected to be weaker, χEFT provides a many-body hierachy.

When evaluating matrix elements, we still encounter integrals that have to be regularized using a cutoff Λ. As this cutoff does not have any physical meaning, low-energy physics should be independent of it. An in-depth review on χEFT with a detailed explanation of chiral symmetry has been written by Machleidt and Entem [20]. In this work we use the two-body interaction at N^{3}LO by Entem and Machleidt [23]. For the three-body interaction, we only include the N^{2}LO contributions by Navrátil [24] with a cutoff of $\Lambda = 500$ MeV.

3 Mathematical Basics

In the following chapter we discuss all the relevant mathematical basics that are needed throughout this work. We start by discussing angular momentum coupling, especially the different coupling possibilities and transformations between them. Furthermore, we discuss coordinate transformations for two-body HO states, a crucial requirement for coordinate transformations in HO bases with more than two particles.

3.1 Angular Momentum Coupling

For the description of a particle with an angular momentum, we use a basis that is created from the eigenstates of the angular momentum operators $\vec{j}^2$ and j_z. The quantum numbers corresponding to these operators are the angular momentum j and the angular momentum projection m_j. For two or more angular momenta, we can choose from different bases.

For instance, for two angular momentum we have an uncoupled basis,

$$\left|j_1 m_{j_1}, j_2 m_{j_2}\right\rangle, \tag{3.1}$$

and a coupled one

$$\left|\left(j_1 j_2\right) J M_J\right\rangle, \tag{3.2}$$

where we indicate the coupling using parantheses. For more than two angular momenta we even have different coupled bases to choose from. The following sections discuss the possible transformations between these bases. We start with the Clebsch-Gordan coefficients (CGCs), which provide a basis transformation between the uncoupled and the coupled two-body basis. Furthermore, 6-J and 9-J symbols are discussed, which are needed for the transformation between different coupled bases of three and four angular momenta, respectively.

3.1.1 Clebsch-Gordan Coefficients

The CGCs connect the coupled and the uncoupled basis,

$$\left|\left(j_1 j_2\right) J M_J\right\rangle = \sum_{m_{j_1}, m_{j_2}} \mathrm{c}\left(\begin{matrix} j_1 & j_2 \\ m_{j_1} & m_{j_2} \end{matrix}\middle| \begin{matrix} J \\ M_J \end{matrix}\right) \left|j_1 m_{j_1}, j_2 m_{j_2}\right\rangle, \tag{3.3}$$

$$\left|j_1 m_{j_1}, j_2 m_{j_2}\right\rangle = \sum_{J, M_J} \mathrm{c}\left(\begin{matrix} j_1 & j_2 \\ m_{j_1} & m_{j_2} \end{matrix}\middle| \begin{matrix} J \\ M_J \end{matrix}\right) \left|\left(j_1 j_2\right) J M_J\right\rangle. \tag{3.4}$$

The CGCs are chosen to be real in this thesis, which ensures that we have the same CGCs for both basis transformations in Eqs. (3.3) and (3.4). To get a non-vanishing CGC some coupling rules must be fulfilled:

$$\mathrm{c}\left(\begin{matrix} j_1 & j_2 \\ m_{j_1} & m_{j_2} \end{matrix}\middle| \begin{matrix} J \\ M_J \end{matrix}\right) = 0 \quad \text{if} \quad \{j_1,\, j_2,\, J\}\, \delta_{m_1+m_2,M} = 0, \tag{3.5}$$

which ensures that the total projection quantum number is the sum of the two projection quantum numbers of the decoupled basis. The angular momenta are restricted by the triangular relation, $\{a,\, b,\, c\}$, which is defined as

$$\{a,\, b,\, c\} = \begin{cases} 1, & \text{if } |a-b| \le c \le a+b \text{ and } a+b+c \text{ is an integer} \\ 0, & \text{otherwise} \end{cases}, \tag{3.6}$$

see p. 85 of Ref. [25]. This relation is symmetric under permutation of its arguments. With these conditions in place the sums in Eqs. (3.3) and (3.4) are finite.

The CGCs fulfill two orthogonality relations used frequently in this thesis to simplify sums over CGCs, see p. 236 of Ref. [25]:

$$\sum_{m_{j_1}, m_{j_2}} \mathrm{c}\left(\begin{matrix} j_1 & j_2 \\ m_{j_1} & m_{j_2} \end{matrix}\middle| \begin{matrix} J \\ M_J \end{matrix}\right) \mathrm{c}\left(\begin{matrix} j_1 & j_2 \\ m_{j_1} & m_{j_2} \end{matrix}\middle| \begin{matrix} J' \\ M'_J \end{matrix}\right) = \delta_{J,J'} \delta_{M_J,M'_J}, \tag{3.7}$$

$$\sum_{J, M_J} \mathrm{c}\left(\begin{matrix} j_1 & j_2 \\ m_{j_1} & m_{j_2} \end{matrix}\middle| \begin{matrix} J \\ M_J \end{matrix}\right) \mathrm{c}\left(\begin{matrix} j_1 & j_2 \\ m'_{j_1} & m'_{j_2} \end{matrix}\middle| \begin{matrix} J \\ M_J \end{matrix}\right) = \delta_{m_{j_1},m'_{j_1}} \delta_{m_{j_2},m'_{j_2}}. \tag{3.8}$$

Furthermore, the following symmetry relations are important, see p. 245 of Ref. [25]:

$$\mathrm{c}\begin{pmatrix} j_1 & j_2 & \\ m_{j_1} & m_{j_2} & \end{pmatrix}\begin{matrix} J \\ M_J \end{matrix} = (-1)^{j_1+j_2-J}\,\mathrm{c}\begin{pmatrix} j_2 & j_1 & \\ m_{j_2} & m_{j_1} & \end{pmatrix}\begin{matrix} J \\ M_J \end{matrix} \tag{3.9}$$

$$= (-1)^{j_1-m_{j_1}}\frac{\hat{J}}{\hat{j}_2}\,\mathrm{c}\begin{pmatrix} J & j_1 & \\ M_J & -m_{j_1} & \end{pmatrix}\begin{matrix} j_2 \\ m_{j_2} \end{matrix}, \tag{3.10}$$

where $\hat{J}$ is a shorthand for $\sqrt{2J+1}$. Note that Eq. (3.9) connects two different coupling orders:

$$\left|\left(j_1 j_2\right) J M_J\right\rangle = (-1)^{j_1+j_2-J}\left|\left(j_2 j_1\right) J M_J\right\rangle. \tag{3.11}$$

3.1.2 6-J Symbols

To convert between different coupling orders of three angular momenta, we need the overlap of the different basis states. This overlap can be calculated using the (Wigner) 6-J symbols. The following transformations are possible, see p. 291 of Ref. [25]:

$$\left|\left[\left(j_1 j_2\right) J_{12} j_3\right] J M_J\right\rangle = \sum_{J_{23}} (-1)^{j_1+j_2+j_3+J}\hat{J}_{12}\hat{J}_{23}\begin{Bmatrix} j_1 & j_2 & J_{12} \\ j_3 & J & J_{23} \end{Bmatrix}\left|\left[j_1\left(j_2 j_3\right) J_{23}\right] J M_J\right\rangle, \tag{3.12}$$

$$\left|\left[\left(j_1 j_2\right) J_{12} j_3\right] J M_J\right\rangle = \sum_{J_{13}} (-1)^{j_2+j_3+J_{12}+J_{13}}\hat{J}_{12}\hat{J}_{13}\begin{Bmatrix} j_2 & j_1 & J_{12} \\ j_3 & J & J_{13} \end{Bmatrix}\left|\left[\left(j_1 j_3\right) J_{13} j_2\right] J M_J\right\rangle, \tag{3.13}$$

$$\left|\left[j_1\left(j_2 j_3\right) J_{23}\right] J M_J\right\rangle = \sum_{J_{13}} (-1)^{j_1+J+J_{23}}\hat{J}_{13}\hat{J}_{23}\begin{Bmatrix} j_1 & j_3 & J_{13} \\ j_2 & J & J_{23} \end{Bmatrix}\left|\left[\left(j_1 j_3\right) J_{13} j_2\right] J M_J\right\rangle, \tag{3.14}$$

where we constructed coupled states with three angular momenta by coupling two of them to an 'intermediate' angular momentum and then couple this angular momentum to a total one. This yields a total angular momentum but it also offers freedom in the coupling order: We can choose which two angular momenta to couple first, yielding all the different possibilities given above. For a state of two angular momenta coupled to a total angular momentum to be physical the three angular momentum quantum numbers need to fulfill the triangular condition and two or none of them can be half-integers. To get a non-vanishing 6-J symbol these conditions must be fulfilled for all four couplings involved in one transformation:

$$\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix} = 0 \quad \text{if} \quad \{a,\,b,\,c\}\{d,\,e,\,c\}\{d,\,b,\,f\}\{a,\,e,\,f\} = 0, \tag{3.15}$$

With these conditions the sums in Eqs. (3.12) to (3.14) are finite. Note that these equations only have one sum each, as the overlap preserves j_1, j_2, j_3, the total angular momentum J and the projection quantum number M_J. To calculate a 6-J symbol the overlap can be written by explicitly decoupling the three angular momenta. This yields the following expression,

$$\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix} = (-1)^{a+b+d+e}\hat{e}\hat{f}\sum_{\substack{m_a,m_b,m_c \\ m_d,m_f}} \mathrm{c}\begin{pmatrix} a & b & \\ m_a & m_b & \end{pmatrix}\begin{matrix} c \\ m_c \end{matrix}\mathrm{c}\begin{pmatrix} c & d & \\ m_c & m_d & \end{pmatrix}\begin{matrix} e \\ m_e \end{matrix}$$
$$\mathrm{c}\begin{pmatrix} b & d & \\ m_b & m_d & \end{pmatrix}\begin{matrix} f \\ m_f \end{matrix}\mathrm{c}\begin{pmatrix} a & f & \\ m_a & m_f & \end{pmatrix}\begin{matrix} e \\ m_e \end{matrix}, \tag{3.16}$$

which connects 6-J symbols with the CGCs, see p. 291 of Ref. [25]. As CGCs are chosen to be real, the 6-J symbols are real-valued as well. Additionally, this ensures that the transformations given in Eqs. (3.12) to (3.14) can be inverted using the same expression for the overlap. The 6-J symbol is invariant under exchange of two columns and under exchange of two angular momenta from the upper row with the angular momenta beneath them, e.g.,

$$\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix} = \begin{Bmatrix} d & e & c \\ a & b & f \end{Bmatrix} = \begin{Bmatrix} d & b & f \\ a & e & c \end{Bmatrix} = \begin{Bmatrix} b & a & c \\ e & d & f \end{Bmatrix} = \begin{Bmatrix} d & f & b \\ a & c & e \end{Bmatrix}. \tag{3.17}$$

For more symmetry relations and explicit formulae for the 6-J symbols see Ref. [25].

3.1.3 9-J Symbols

The Wigner 9-J symbols (also called Fano coefficients) are used for changing the coupling scheme of four angular momenta. We can express the overlap of the basis states of different coupling schemes in terms of 9-J symbols, see p. 334 of Ref. [25]:

$$\left|\left[\left(j_1 j_2\right) J_{12}\left(j_3 j_4\right) J_{34}\right] J M_J\right\rangle = \sum_{J_{13},\,J_{24}} \hat{J}_{12}\hat{J}_{34}\hat{J}_{13}\hat{J}_{24} \begin{Bmatrix} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{Bmatrix} \left|\left[\left(j_1 j_3\right) J_{13}\left(j_2 j_4\right) J_{24}\right] J M_J\right\rangle, \tag{3.18}$$

$$\left|\left[\left(j_1 j_2\right) J_{12}\left(j_3 j_4\right) J_{34}\right] J M_J\right\rangle = \sum_{J_{14},\,J_{23}} \hat{J}_{12}\hat{J}_{34}\hat{J}_{14}\hat{J}_{23}(-1)^{j_3+j_4-J_{34}} \begin{Bmatrix} j_1 & j_2 & J_{12} \\ j_4 & j_3 & J_{34} \\ J_{14} & J_{23} & J \end{Bmatrix} \left|\left[\left(j_1 j_4\right) J_{14}\left(j_2 j_3\right) J_{23}\right] J M_J\right\rangle, \tag{3.19}$$

$$\left|\left[\left(j_1 j_3\right) J_{13}\left(j_2 j_4\right) J_{24}\right] J M_J\right\rangle = \sum_{J_{14},\,J_{23}} \hat{J}_{13}\hat{J}_{24}\hat{J}_{14}\hat{J}_{23}(-1)^{j_3-j_4+J_{24}-J_{23}} \begin{Bmatrix} j_1 & j_3 & J_{13} \\ j_4 & j_2 & J_{24} \\ J_{14} & J_{23} & J \end{Bmatrix} \left|\left[\left(j_1 j_4\right) J_{14}\left(j_2 j_3\right) J_{23}\right] J M_J\right\rangle. \tag{3.20}$$

The same recoupling could be achieved by using multiple 6-J symbols, therefore we can express a 9-J symbol in terms of 6-J symbols, see p. 340 of Ref. [25]:

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} = \sum_K (-1)^{2K}\hat{K} \begin{Bmatrix} a & b & c \\ f & i & K \end{Bmatrix} \begin{Bmatrix} d & e & f \\ b & K & h \end{Bmatrix} \begin{Bmatrix} g & h & i \\ K & a & d \end{Bmatrix}. \tag{3.21}$$

As the 6-J symbols are real, the same is valid for the 9-J symbols. Therefore the transformations given in Eqs. (3.18) to (3.20) can be inverted using the same expression for the overlap.

To get a non-vanishing 9-J symbol the triangular condition must be fulfilled for every row and every column. Furthermore there can only be two or none half-integer numbers per row and per column. The 9-J symbol is symmetric under even permutations of rows and columns and it yields a factor of $(-1)^{a+b+c+d+e+f+g+h+i}$ for odd permutations. For more symmetries and explicit formulae for 9-J symbols see Ref. [25].

3.1.4 Sums of Coupling Coefficients

The following formulae are used to simplify expressions involving 6-J and 9-J symbols. All of these relations and many more have been summarized by Varshalovich et al., see pp. 462 - 474 of Ref. [25]. Only the ones that are used in this work are listed here.

$$\sum_K (2K+1) \begin{Bmatrix} a & b & K \\ c & d & e \end{Bmatrix} \begin{Bmatrix} c & d & K \\ a & b & f \end{Bmatrix} = \frac{\delta_{e,f}}{2f+1} \{a,\, d,\, e\} \{c,\, b,\, e\}, \tag{3.22}$$

$$\sum_K (-1)^K (2K+1) \begin{Bmatrix} a & b & K \\ c & d & e \end{Bmatrix} \begin{Bmatrix} c & d & K \\ b & a & f \end{Bmatrix} = (-1)^{e+f} \begin{Bmatrix} a & d & e \\ b & c & f \end{Bmatrix}, \tag{3.23}$$

$$\sum_K (2K+1) \begin{Bmatrix} a & b & p \\ c & d & q \\ r & s & K \end{Bmatrix} \begin{Bmatrix} e & f & p \\ g & h & q \\ r & s & K \end{Bmatrix} = (-1)^{b+g+r+s-c-f-p-q} \sum_{K'} (2K'+1) \begin{Bmatrix} a & p & b \\ r & e & g \\ c & f & K' \end{Bmatrix} \begin{Bmatrix} d & s & b \\ q & h & g \\ c & f & K' \end{Bmatrix}, \tag{3.24}$$

$$\sum_K (2K+1) \begin{Bmatrix} a & f & K \\ d & q & e \\ p & c & b \end{Bmatrix} \begin{Bmatrix} a & f & K \\ e & b & s \end{Bmatrix} = (-1)^{2s} \begin{Bmatrix} a & b & s \\ c & d & p \end{Bmatrix} \begin{Bmatrix} c & d & s \\ e & f & q \end{Bmatrix}. \tag{3.25}$$

3.2 Coordinate Transformations

For the coordinate transformation we have got a two particle HO basis, where the two states are coupled to a total orbital angular momentum:

$$\left|\left[n_1 l_1(\vec{r}_1), n_2 l_2(\vec{r}_2)\right] \Lambda M_\Lambda\right\rangle, \tag{3.26}$$

where n_1 and n_2 indicate radial quantum numbers while l_1 and l_2 are orbital angular momentum quantum numbers of the HO states. The coordinate vectors $\vec{r}_1$ and $\vec{r}_2$ indicate that the quantum numbers are defined with respect to these coordinates. Usually the underlying coordinate system is unambigious and, therefore, these coordinate labels are omitted to avoid confusion with the coordinate representation of these states. The coordinates can, for example, be single-particle coordinates, also called absolute coordinates. In this case n_1 and l_1 are quantum numbers of the first particle, while n_2 and l_2 belong to the second particle. However, this is not necessarily the case. The two orbital angular momenta are coupled to a total orbital angular momentum Λ. For coupled states the following notation is used in this thesis: The two angular momenta that are coupled are in parantheses followed by the total angular momentum.

We want to construct a basis that is defined with respect to a different set of coordinates, e.g., center-of-mass coordinates, which are denoted by $\vec{R}$ and $\vec{r}$:

$$\left|\left[NL(\vec{R}), nl(\vec{r})\right] \Lambda' M'_\Lambda\right\rangle, \tag{3.27}$$

where we have the radial quantum numbers N and n as well as the orbital angular momenta L and l. We assume that the transformation between the two sets of coordinates can be described with the following matrix

$$\begin{pmatrix}\vec{R}\\ \vec{r}\end{pmatrix} = \begin{pmatrix}\sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}}\\ \sqrt{\frac{1}{1+d}} & -\sqrt{\frac{d}{1+d}}\end{pmatrix}\begin{pmatrix}\vec{r}_1\\ \vec{r}_2\end{pmatrix}, \tag{3.28}$$

which is symmetric and unitary and only depends on one parameter d. The transformation between the two bases can be written as

$$\begin{aligned}\left|\left[NL(\vec{R}), nl(\vec{r})\right] \Lambda' M'_\Lambda\right\rangle = \sum_{\Lambda, M_\Lambda} \sum_{n_1, l_1, n_2, l_2} &\left\langle \left[n_1 l_1(\vec{r}_1), n_2 l_2(\vec{r}_2)\right] \Lambda M_\Lambda \middle| \left[NL(\vec{R}), nl(\vec{r})\right] \Lambda' M'_\Lambda \right\rangle \\ &\left|\left[n_1 l_1(\vec{r}_1), n_2 l_2(\vec{r}_2)\right] \Lambda M_\Lambda\right\rangle,\end{aligned} \tag{3.29}$$

where the overlap between the two basis states is given by a harmonic-oscillator bracket (HOB) as defined by Kamuntavičius et al. [26]:

$$\left\langle \left[n_1 l_1(\vec{r}_1), n_2 l_2(\vec{r}_2)\right] \Lambda M_\Lambda \middle| \left[NL(\vec{R}), nl(\vec{r})\right] \Lambda' M'_\Lambda \right\rangle = \delta_{\Lambda,\Lambda'} \delta_{M_\Lambda, M'_\Lambda} \ll n_1 l_1, n_2 l_2 | NL, nl; \Lambda \gg_d . \tag{3.30}$$

The HOBs have some important properties that are advantageous for an actual calculation. As can be seen from Eq. (3.30), the coordinate transformation is independent of the projection quantum number M_Λ and it does not change the total angular momentum Λ. Furthermore the HOB enforces energy conservation of the states involved, yielding

$$2N + L + 2n + l = 2n_1 + l_1 + 2n_2 + l_2. \tag{3.31}$$

This property ensures that the sum in Eq. (3.29) is finite. Additionally the HOBs obey the following symmetry relations:

$$\ll n_1 l_1, n_2 l_2 | NL, nl; \Lambda \gg_d = \ll NL, nl | n_1 l_1, n_2 l_2; \Lambda \gg_d \tag{3.32}$$

$$= (-1)^{L-\Lambda} \ll n_2 l_2, n_1 l_1 | NL, nl; \Lambda \gg_{\frac{1}{d}} \tag{3.33}$$

$$= (-1)^{l_1-\Lambda} \ll n_1 l_1, n_2 l_2 | nl, NL; \Lambda \gg_{\frac{1}{d}} \tag{3.34}$$

$$= (-1)^{l_2+L} \ll n_2 l_2, n_1 l_1 | nl, NL; \Lambda \gg_d . \tag{3.35}$$

Equation (3.32) follows from the fact that we have got a real, symmetric and unitary matrix. Therefore the inverse coordinate transformation must be the same as the original one and the value of the harmonic-oscillator bracket

is identical. As the inverse HOB must be the complex conjugate of the original one this property also ensures real-valued HOBs.

To derive Eq. (3.33) we use that Eq. (3.28) can also be written as

$$\begin{pmatrix} \vec{R} \\ -\vec{r} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{1+d}} & \sqrt{\frac{d}{1+d}} \\ \sqrt{\frac{d}{1+d}} & -\sqrt{\frac{1}{1+d}} \end{pmatrix} \begin{pmatrix} \vec{r}_2 \\ \vec{r}_1 \end{pmatrix}, \tag{3.36}$$

where the transformation matrix has been established by substituting d with $1/d$. We use the coordinate representation of the transformation to establish the connection:

$$\begin{aligned}
&\ll n_1 l_1, n_2 l_2 | NL, nl; \Lambda \gg_d \\
&= \left\langle \left[n_1 l_1(\vec{r}_1), n_2 l_2(\vec{r}_2) \right] \Lambda M_\Lambda \right| \left[NL(\vec{R}), nl(\vec{r}) \right] \Lambda M_\Lambda \rangle && (3.37) \\
&= \sum_{m_{l_1}, m_{l_2}} \mathrm{c} \begin{pmatrix} l_1 & l_2 & \Lambda \\ m_{l_1} & m_{l_2} & M_\Lambda \end{pmatrix} \sum_{m_L, m_l} \mathrm{c} \begin{pmatrix} L & l & \Lambda \\ m_L & m_l & M_\Lambda \end{pmatrix} \\
&\quad \int d^3\vec{r}_1 \int d^3\vec{r}_2 \Phi^*_{n_1,l_1}(\vec{r}_1)\, \Phi^*_{n_2,l_2}(\vec{r}_2)\, \Phi_{N,L}\left(\vec{R}\right) \Phi_{n,l}(\vec{r}) && (3.38) \\
&= (-1)^{l_1+l_2-\Lambda} (-1)^l \sum_{m_{l_2}, m_{l_1}} \mathrm{c} \begin{pmatrix} l_2 & l_1 & \Lambda \\ m_{l_2} & m_{l_1} & M_\Lambda \end{pmatrix} \sum_{m_L, m_l} \mathrm{c} \begin{pmatrix} L & l & \Lambda \\ m_L & m_l & M_\Lambda \end{pmatrix} \\
&\quad \int d^3\vec{r}_1 \int d^3\vec{r}_2 \Phi^*_{n_2,l_2}(\vec{r}_2)\, \Phi^*_{n_1,l_1}(\vec{r}_1)\, \Phi_{N,L}\left(\vec{R}\right) \Phi_{n,l}(-\vec{r}) && (3.39) \\
&= (-1)^{l_1+l_2-\Lambda} (-1)^l \left\langle \left[n_2 l_2(\vec{r}_2), n_1 l_1(\vec{r}_1) \right] \Lambda M_\Lambda \right| \left[NL(\vec{R}), nl(-\vec{r}) \right] \Lambda M_\Lambda \rangle && (3.40) \\
&= (-1)^{L-\Lambda} \ll n_2 l_2, n_1 l_1 | NL, nl; \Lambda \gg_{\frac{1}{d}}, && (3.41)
\end{aligned}$$

where $\Phi_{n,l}(\vec{r})$ are normalized HO wave functions. The choice of M_Λ is arbitrary as long as the resulting states are physical. It does not have any effect on the symmetry relation and the HOB does not depend on it. The phase in Eq. (3.39) emerges from the reordering of the coupling $(-1)^{l_1+l_2-\Lambda}$ and the parity transformation of the wave function $(-1)^l$. Equations (3.34) and (3.35) can be obtained by combining the first two symmetry relations.

Furthermore, an orthogonality relation can be found for the HOBs, see Eq. (21) of Ref. [26]:

$$\sum_N \sum_L \sum_n \sum_l \ll n_1 l_1, n_2 l_2 | NL, nl; \Lambda \gg_d \ll NL, nl | n_1' l_1', n_2' l_2'; \Lambda \gg_d = \delta_{n_1,n_1'} \delta_{n_2,n_2'} \delta_{l_1,l_1'} \delta_{l_2,n_2'}, \tag{3.42}$$

which ensures that we get the original state again, if we apply the coordinate transformation twice. The formula follows directly from the orthogonality and the normalization of the HO basis.

An efficient formula for calculating HOBs has been proposed by Kamuntavičius et al., see Eq. (26) of Ref. [26], where a phase modification of $(-1)^{N+n+n_1+n_2}$ must be applied, as our definition of the HO wave function is different. For a discussion of the phase modification or an in-depth discussion of symmetries see Ref. [26]. Be aware of alternative definitions of HOBs that lead to different formulae and different symmetry relations [27, 28].

4 Bases

In this chapter we discuss the different bases that are used in this work. These are the Jacobi basis for two, three and four particles, as well as the m-scheme and the JT-coupled scheme. Furthermore we discuss advantages and disadvantages of the different bases as well as multiple transformations between them: We need to be able to transform matrix elements from the Jacobi basis to the JT-coupled scheme. Moreover, we introduce the partial-trace approximation, which reduces matrix elements that are given in four-body Jacobi basis to matrix elements in three-body Jacobi basis. Finally, we discuss the transformation of matrix elements from a given basis to a basis with more particles.

4.1 Jacobi Basis

The Jacobi basis is defined with respect to Jacobi coordinates, which we will discuss first. We then use these coordinates to construct the basis for two, three and four particles.

4.1.1 Coordinate System

Jacobi coordinates are a generalization of two-body relative coordinates for more than two particles with identical mass:

$$\vec{\xi}_0 = \sqrt{\frac{1}{N}} \left(\vec{r}_1 + \ldots + \vec{r}_N\right), \tag{4.1}$$

$$\vec{\xi}_1 = \sqrt{\frac{1}{2}} \left(\vec{r}_1 - \vec{r}_2\right), \tag{4.2}$$

$$\vec{\xi}_k = \sqrt{\frac{k}{k+1}} \left[\frac{1}{k}\left(\vec{r}_1 + \ldots + \vec{r}_k\right) - \vec{r}_{k+1}\right], \tag{4.3}$$

where we have N particles with absolute coordinates $\vec{r}_1, \ldots, \vec{r}_N$ and Jacobi coordinates $\vec{\xi}_0, \ldots, \vec{\xi}_{N-1}$. Note that these coordinates are only one choice for Jacobi coordinates and there exist different possibilities.

The zeroth Jacobi coordinate $\vec{\xi}_0$ is always proportional to the center of mass of all particles and the first coordinate $\vec{\xi}_1$ is proportional to the distance between the first two particles, similar to the standard relative coordinates. The remaining coordinates are all proportional to the distance of the next particle to the center-of-mass of the previous particles. An illustration of the construction of the Jacobi coordinates can be found in Fig. 4.1.

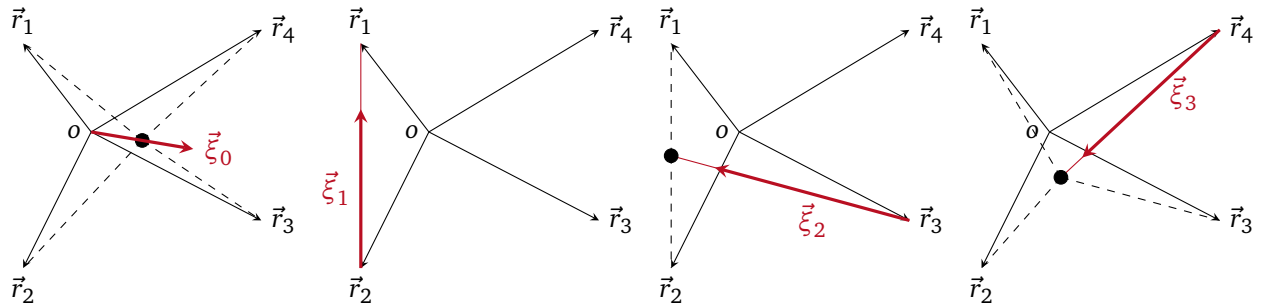


Figure 4.1: Construction of four-body Jacobi coordinates from absolute coordinates. The absolute coordinates are denoted by $\vec{r}_1$, $\vec{r}_2$, $\vec{r}_3$ and $\vec{r}_4$, while $\vec{\xi}_0$, $\vec{\xi}_1$, $\vec{\xi}_2$ and $\vec{\xi}_3$ indicate Jacobi coordinates. Filled circles represent the center-of-mass of the particles connected by dashed lines. The origin is marked by o.

A very important property of this choice of coordinates is the structure of the harmonic-oscillator Hamiltonian in these coordinates. It shows the same structure as in the case of absolute coordinates, e.g., the four-body Hamiltonian in both coordinates yields:

$$\begin{aligned} H &= \frac{\vec{p}_1^{\,2}}{2m} + \tfrac{1}{2}m\omega^2\vec{r}_1 + \frac{\vec{p}_2^{\,2}}{2m} + \tfrac{1}{2}m\omega^2\vec{r}_2 + \frac{\vec{p}_3^{\,2}}{2m} + \tfrac{1}{2}m\omega^2\vec{r}_3 + \frac{\vec{p}_4^{\,2}}{2m} + \tfrac{1}{2}m\omega^2\vec{r}_4 \\ &= \frac{\vec{\pi}_0^{\,2}}{2m} + \tfrac{1}{2}m\omega^2\vec{\xi}_0 + \frac{\vec{\pi}_1^{\,2}}{2m} + \tfrac{1}{2}m\omega^2\vec{\xi}_1 + \frac{\vec{\pi}_2^{\,2}}{2m} + \tfrac{1}{2}m\omega^2\vec{\xi}_2 + \frac{\vec{\pi}_3^{\,2}}{2m} + \tfrac{1}{2}m\omega^2\vec{\xi}_3, \end{aligned} \tag{4.4}$$

where the coordinates and momenta are operators. The momenta can be transformed from absolute momenta ($\vec{p}_1$, $\vec{p}_2$, $\vec{p}_3$, $\vec{p}_4$) to Jacobi ones ($\vec{\pi}_0$, $\vec{\pi}_1$, $\vec{\pi}_2$, $\vec{\pi}_3$) by using the same formulae that we used for the coordinates themselves (Eqs. 4.1 – 4.3). As the algebraic structure of the Hamiltonian is preserved, the solutions to the time-independent Schrödinger equation are identical as well. There is just one difference, the eigenstates to H are defined with respect to different coordinates.

4.1.2 Two-Body Basis

Using these Jacobi coordinates we construct a quantum mechanical basis using HO states. For two bodies this is rather simple:

$$\left|N_{\mathrm{cm}} L_{\mathrm{cm}} M_{L_{\mathrm{cm}}}; N_1; (L_1 S_1) J_1 M_{J_1}; T_1 M_{T_1}\right\rangle . \tag{4.5}$$

In the Jacobi basis, the lower index indicates the Jacobi coordinate this quantum number corresponds to, e.g., N_{cm} is the radial quantum number corresponding to the zeroth Jacobi coordinate and L_1 is the orbital angular momentum that is defined with respect to the first Jacobi coordinate. All quantum numbers that correspond to multiple particles are indicated using capital letters. As each Jacobi coordinate depends on multiple absolute coordinates, no quantum number in this bases corresponds to just one particle. Of course, Jacobi coordinates do not change spin and isospin. To incorporate them into the scheme, spin and isospin of the first two particles are coupled to a total spin S_1 and total isospin T_1, respectively. The spin is then coupled to the relative orbital angular momentum of the first two particles, yielding a total relative angular momentum J_1. Note that center-of-mass orbital angular momentum, which corresponds to the zeroth Jacobi coordinate, is not coupled to any other angular momentum.

Only basis states that are antisymmetric under exchange of the two particles are of interest to us. We achieve this by explicitly applying the antisymmetrizer to the basis states:

$$\begin{aligned}
&\mathcal{A}\left|N_1; (L_1 S_1) J_1 M_{J_1}; T_1 M_{T_1}\right\rangle \\
&= \frac{1}{2}\left(1 - \tau_{1,2}\right)\left|N_1; (L_1 S_1) J_1 M_{J_1}; T_1 M_{T_1}\right\rangle && (4.6)\\
&= \frac{1}{2}\left(1 - (-1)^{L_1+S_1+T_1}\right)\left|N_1; (L_1 S_1) J_1 M_{J_1}; T_1 M_{T_1}\right\rangle , && (4.7)
\end{aligned}$$

where the center-of-mass part is omitted as it is symmetric by construction and $\tau_{1,2}$ indicates the particle exchange operator. From this equation it directly follows that all states fulfilling the condition

$$(-1)^{L_1+S_1+T_1} = -1 \tag{4.8}$$

are antisymmetric. The $(-1)^{L_1}$ part corresponds to a parity transformation, which is the same as a particle exchange in coordinate space for two particles. The remaining part can be derived easily by expressing the coupled state with decoupled ones and using the symmetry relations of the CGCs (see Eq. 3.9) to exchange the two particles in spin and isospin space.

4.1.3 Three-Body Basis

To get an antisymmetrized three-body basis using Jacobi coordinates we need to invest more effort. We can construct a partially antisymmetrized basis based on the two-body case:

$$\left|N_{\mathrm{cm}} L_{\mathrm{cm}} M_{L_{\mathrm{cm}}}\right\rangle \left|E_{12} J_{12} M_{J_{12}} T_{12} M_{T_{12}} k_{12}\right\rangle = \left|N_{\mathrm{cm}} L_{\mathrm{cm}} M_{L_{\mathrm{cm}}}; N_1 N_2; \left[(L_1 S_1) J_1 \left(L_2 \tfrac{1}{2}\right) J_2\right] J_{12} M_{J_{12}}; \left(T_1 \tfrac{1}{2}\right) T_{12} M_{T_{12}}\right\rangle , \tag{4.9}$$

where the left-hand side will be used as an abbreviation for the full basis state throughout this thesis. For this abbreviation we used the total relative harmonic-oscillator energy $E_{12} = 2N_1 + L_1 + 2N_2 + L_2$. The number k_{12} is used to index all the remaining quantum numbers (N_1, L_1, S_1, J_1, T_1, N_2, L_2 and J_2). The parity of this basis is given by $\pi_{12} = (-1)^{E_{12}} = (-1)^{L_1+L_2}$. To construct this basis we added quantum numbers corresponding to the second Jacobi coordinate, $N_2, L_2 \leftrightarrow \vec{\xi}_2$, to the two-body state. Be aware that the center-of-mass part corresponds to three particles now. Again spin and orbital angular momenta are coupled to a total relative angular momentum and the basis has got a total isospin. The indices for these quantum numbers are constructed in a predictable manner, coupling angular momenta with indices 1 and 2 yields an index of 12.

The basis is already antisymmetric under exchange of the first two particles if Eq. (4.8) is fulfilled. For constructing a fully antisymmetric basis, we need to explicitly antisymmetrize the basis given above by calculating the matrix elements of the antisymmetrizing operator. As the center-of-mass part is always symmetric only the relative part is relevant. The operator does not have any effect on the projection quantum numbers, therefore we will omit them in the following formulae. The antisymmetrizer turns out to be a block-diagonal matrix when represented in the three-body Jacobi basis,

$$\left\langle E'_{12}J'_{12}T'_{12}k'_{12}\right|\mathcal{A}\left|E_{12}J_{12}T_{12}k_{12}\right\rangle = \begin{pmatrix} \boxed{E,J,T} & & \\ & \boxed{E',J',T'} & \\ & & \ddots \end{pmatrix}, \tag{4.10}$$

where each block corresponds to a given energy, total isospin and total relative angular momentum. We can now extract the antisymmetric states by diagonalizing the matrix. Because antisymmetric states do not change when applying the antisymmetrizing operator, they can be identified with the eigenstates to the eigenvalue 1 for the matrix given above. Any eigenstate to the eigenvalue 0 does not have a well-defined symmetry and is omitted. Each block is diagonalized separately and for each block there can be multiple eigenstates that correspond to the eigenvalue 1. We will label these eigenstates by i_{12}. Using the eigenvectors for the basis transformation, the antisymmetric state can now be expressed by the partially antisymmetric ones.

$$\left|E_{12}i_{12}J_{12}T_{12}\right\rangle_a = \sum_{k_{12}} c_{k_{12}}^{E_{12},J_{12},T_{12},i_{12}} \left|E_{12}J_{12}T_{12}k_{12}\right\rangle, \tag{4.11}$$

where $c_{k_{12}}^{E_{12},J_{12},T_{12},i_{12}}$ is a coefficient of fractional parentage (CFP) [29], it is simply the k_{12}-th entry of the i_{12}-th eigenvector of the block indicated by E_{12}, J_{12} and T_{12}.

For a derivation of the formula for the antisymmetrizing operator matrix elements,

$$\begin{aligned}
&\left\langle E'_{12}J'_{12}T'_{12}k'_{12}\right|\mathcal{A}\left|E_{12}J_{12}T_{12}k_{12}\right\rangle \\
&\quad=\delta_{E_{12},E'_{12}}\delta_{J_{12},J'_{12}}\delta_{T_{12},T'_{12}}\Bigg(\tfrac{1}{3}\delta_{k_{12},k'_{12}} - \tfrac{2}{3}\sum_{L,S}(-1)^{S_1+S'_1+T_1+T'_1}\hat{L}^2\hat{S}^2\hat{J}_1\hat{J}'_1\hat{J}_2\hat{J}'_2\hat{S}_1\hat{S}'_1\hat{T}_1\hat{T}'_1 \\
&\qquad\qquad \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S'_1 \\ \frac{1}{2} & S & S_1 \end{Bmatrix}\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & T'_1 \\ \frac{1}{2} & T_{12} & S_1 \end{Bmatrix}\begin{Bmatrix} L_1 & S_1 & J_1 \\ L_2 & \frac{1}{2} & J_2 \\ L & S & J_{12} \end{Bmatrix}\begin{Bmatrix} L'_1 & S'_1 & J'_1 \\ L'_2 & \frac{1}{2} & J'_2 \\ L & S & J_{12} \end{Bmatrix} \\
&\qquad\qquad \ll N'_1L'_1,N'_2L'_2|N_1L_1,N_2L_2;L\gg_{\frac{1}{3}}\Bigg),
\end{aligned} \tag{4.12}$$

see pp. 128 - 143 of Ref. [11].

4.1.4 Four-Body Basis

For the four-body Jacobi basis we use the same approach as for the three-body one. We will first define a partially antisymmetric basis,

$$\begin{aligned}
&\left|N_{\mathrm{cm}}L_{\mathrm{cm}}M_{L_{\mathrm{cm}}}\right\rangle\left|E_{123}J_{123}M_{J_{123}}T_{123}M_{T_{123}}k_{123}\right\rangle \\
&\quad=\left|N_{\mathrm{cm}}L_{\mathrm{cm}}M_{L_{\mathrm{cm}}};E_{12}i_{12}N_3;\left[J_{12}\left(L_3\tfrac{1}{2}\right)J_3\right]J_{123}M_{J_{123}};\left(T_{12}\tfrac{1}{2}\right)T_{123}M_{T_{123}}\right\rangle,
\end{aligned} \tag{4.13}$$

which is based on the three-body basis. The center-of-mass is now defined with respect to four particles and we introduced a total relative energy $E_{123} = E_{12} + 2N_3 + L_3$. The left hand side of the equation will be used as an abbreviation for a basis state, where k_{123} is used to index the remaining quantum numbers (E_{12}, J_{12}, T_{12}, i_{12}, N_3, L_3 and J_3). Additionally, a quantum number for parity is introduced: $\pi_{123} = (-1)^{E_{123}}$.

Again, the basis is antisymmetric with respect to the first three particles and we have to calculate the antisymmetrizing operator to get a fully antisymmetric basis. The operator does not act on the projection quantum numbers and the matrix is a block-diagonal one, where the blocks are defined by E_{123}, J_{123} and T_{123}:

$$\begin{aligned}
&\left\langle E'_{123}J'_{123}T'_{123}k'_{123}\right|\mathcal{A}\left|E_{123}J_{123}T_{123}k_{123}\right\rangle \\
&=\delta_{E_{123},E'_{123}}\delta_{J_{123},J'_{123}}\delta_{T_{123},T'_{123}}\Bigg(\tfrac{1}{4}\delta_{k_{123},k'_{123}}-\tfrac{3}{4}\sum_{k_{12},k'_{12}}\sum_{L_{23},K}c_{k_{12}}^{E_{12},J_{12},T_{12},i_{12}}\hat{J}_{12}\hat{J}_2\hat{J}_3\hat{L}_{23}^2\hat{T}_{12}\hat{J}'_{12}\hat{J}'_2\hat{J}'_3\hat{T}'_{12}\hat{K}^2 \\
&\qquad(-1)^{T_{12}+T'_{12}+L_2+L'_2+J_2+J'_2}\delta_{N_1,N'_1}\delta_{L_1,L'_1}\delta_{S_1,S'_1}\delta_{J_1,J'_1}\delta_{T_1,T'_1} \\
&\qquad\begin{Bmatrix}J_1 & J_2 & J_{12}\\ J'_2 & K & J_3\\ J'_{12} & J'_3 & J_{123}\end{Bmatrix}\begin{Bmatrix}L'_2 & L_3 & K\\ J_3 & J'_2 & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix}L_2 & L'_3 & K\\ J'_3 & J_2 & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix}L_3 & L'_2 & K\\ L'_3 & L_2 & L_{23}\end{Bmatrix} \\
&\qquad\begin{Bmatrix}\frac{1}{2} & T_{123} & T_{12}\\ \frac{1}{2} & T_1 & T'_{12}\end{Bmatrix}\ll N'_2L'_2,N'_3L'_3|N_2L_2,N_3L_3;L_{23}\gg_{\frac{1}{8}}\Bigg).
\end{aligned}\tag{4.14}$$

The derivation can be found in appendix A. We can diagonalize this matrix and express the completely antisymmetric state with the partially antisymmetric one using four-body CFPs:

$$\left|E_{123}i_{123}J_{123}T_{123}\right\rangle_a=\sum_{k_{123}}\tilde{c}_{k_{123}}^{E_{123},J_{123},T_{123},i_{123}}\left|E_{123}J_{123}T_{123}k_{123}\right\rangle,\tag{4.15}$$

where the number i_{123} is used to label the antisymmetric states.

4.2 m-Scheme Basis

The m-scheme basis consists of Slater-determinants of single-particle harmonic-oscillator states. A four-body state would be written as

$$\left|abcd\right\rangle_a=\sqrt{4!}\mathcal{A}\left|n_a;\left(l_a\tfrac{1}{2}\right)j_am_{j_a};\tfrac{1}{2}m_{t_a}\right\rangle\left|n_b;\left(l_b\tfrac{1}{2}\right)j_bm_{j_b};\tfrac{1}{2}m_{t_b}\right\rangle\left|n_c;\left(l_c\tfrac{1}{2}\right)j_cm_{j_c};\tfrac{1}{2}m_{t_c}\right\rangle\left|n_d;\left(l_d\tfrac{1}{2}\right)j_dm_{j_d};\tfrac{1}{2}m_{t_d}\right\rangle,\tag{4.16}$$

with harmonic-oscillator states that are defined with respect to the absolute coordinates of the four particles. The left-hand side of Eq. (4.16) will be used as an abbreviation for the m-scheme state throughout this thesis. In this basis the indices correspond to the particles a to d and we use lower-case letters for the quantum numbers, as all of them correspond to a single particle. The total HO energy quantum number is given by

$$E=2n_a+l_a+2n_b+l_b+2n_c+l_c+2n_d+l_d.\tag{4.17}$$

This basis can easily be constructed for any number of particles and for this reason it is convenient for many-body calculations. This state does not have a good quantum number with respect to total isospin or total angular momentum, however, it has good quantum numbers with respect to the projection of total isospin or total angular momentum on the z-axis. They are given by the sums of the projection quantum numbers,

$$M_T=\sum_i m_{t_i},\tag{4.18}$$

$$M_J=\sum_i m_{j_i},\tag{4.19}$$

hence the name 'm-scheme'.

A basis with total angular momentum and total isospin can be constructed by coupling the angular momenta and the isospin to a total angular momentum and total isospin, respectively, e.g.,

$$\begin{aligned}
&\left|EJM_JTM_T\alpha_{abcd}\right\rangle_a \\
&=\left|n_an_bn_cn_d;\left\{\left\{\left[\left(l_a\tfrac{1}{2}\right)j_a\left(l_b\tfrac{1}{2}\right)j_b\right]J_{ab}\left(l_c\tfrac{1}{2}\right)j_c\right\}J_{abc}\left(l_d\tfrac{1}{2}\right)j_d\right\}JM_J;\left\{\left[\left(\tfrac{1}{2}\tfrac{1}{2}\right)T_{ab}\tfrac{1}{2}\right]T_{abc}\tfrac{1}{2}\right\}TM_T\right\rangle_a,
\end{aligned}\tag{4.20}$$

for a four-body state. We again introduce a shorthand for the state using α_{abcd} to label the quantum numbers n_a, n_b, n_c, n_d, l_a, l_b, l_c, l_d, j_a, j_b, j_c, j_d, J_{ab}, J_{abc}, T_{ab} and T_{abc}. This basis is called the JT-coupled scheme. Again all quantum numbers that are constructed by coupling multiple angular momentum or isospin quantum numbers are written in capital letters. Note that the basis states are neither orthogonal nor normalized. The normalization constant is chosen in such a way that we obtain an orthonormal m-scheme basis simply by decoupling the JT-coupled scheme.

4.3 Comparison of Harmonic-Oscillator Bases

When choosing a specific basis to construct a model space it is important to take the symmetries of the Hamiltonian into account. In this thesis we generally select a model space by using an energy truncation, e.g., we only include m-scheme states with $E \leq E_{\text{max}}$. In principle, the model space constructed using the m-scheme, the JT-coupled scheme or the Jacobi basis have the same size for the same energy truncation. However, because of the symmetries of the Hamiltonian, some of the matrix elements in the model spaces are redundant. The Hamiltonian is, for instance, invariant under rotations. Such a continuous symmetry generates a conserved quantity, which is angular momentum in this case. When representing the Hamiltonian in a basis with a total angular momentum, the conservation law ensures a matrix representation that is diagonal in angular momentum. As all off-diagonal terms are 0 it is not necessary to store them, which reduces the storage space needed for representing the Hamiltonian in this basis.

Considering these symmetries, representing the Hamiltonian in the Jacobi basis requires the smallest storage space, as numerous properties of our interaction can be used:

- Translational invariance ensures that the Hamiltonian is independent of all center-of-mass quantum numbers.
- Rotational invariance ensures a Hamiltonian that is diagonal in total relative angular momentum, i.e., J_{123} and $M_{J_{123}}$ in the four-body case. Additionally, the Hamiltonian is independent of the total relative angular-momentum projection quantum number, e.g. $M_{J_{12}}$ or $M_{J_{123}}$ in the three- or four-body case, respectively.
- Isospin symmetry for three or more particles ensures a Hamiltonian that is diagonal in total isospin, i.e., T_{123} and $M_{T_{123}}$ in the four-body case. Additionally, the Hamiltonian is independent of $M_{T_{12}}$ or $M_{T_{123}}$ in the three- or four-body case, respectively.
- The Hamiltonian does not change the parity of the states.

The isospin symmetry is an approximation that is applied in the three- and four-body case. In the two-body case, the differences between different total isospin projections are taken into account, as they are relevant for the description of nuclei. Three- and four-body contributions are generally weaker than the two-body ones and the effects of the isospin projection are negligible. Note that the energy truncation in the Jacobi basis can be applied to the total relative HO energy, e.g., $E_{123} \leq E_{\text{max}}$ for the four-body basis, as the Hamiltonian is independent of the center-of-mass part.

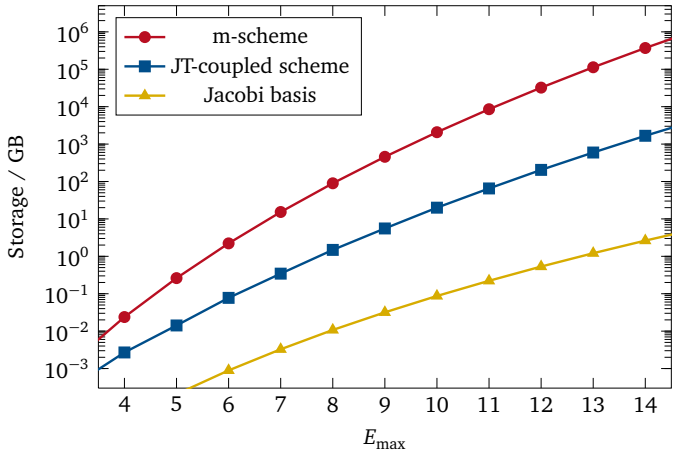


Figure 4.2: Storage space needed for four-body matrix elements in different HO representations over the energy truncation when using 8 bytes for each matrix element. The energy truncation of the Jacobi basis only applies to the relative energies as the center-of-mass part is omitted. Lines are included to guide the eye.

While the Jacobi basis seems to be perfect for storing the Hamiltonian, a many-body Jacobi basis cannot be constructed, as the explicit calculation of the antisymmetrization operator is not feasible for a many-body basis. The m-scheme, on the other hand, can be constructed easily for any number of particles and it is, therefore, the basis used in a subsequent many-body calculation. However, as it does not have center-of-mass, total angular momentum or total isospin quantum numbers, all the according symmetries cannot be used to reduce the storage space.

To rectify this disadvantage, we can use the JT-coupled scheme, which has a total isospin and total angular momentum and thus needs less storage space. As the many-body methods require the m-scheme, the states are decoupled on-the-fly during the many-body calculation to avoid storing the Hamiltonian in a m-scheme representation. A comparison of the storage space needed for the different representations of the Hamiltonian is presented in Fig. 4.2.

4.4 Jacobi Basis to JT-coupled Scheme

In the following chapter we derive the basis transformation from a four-body Jacobi basis to the four-body JT-coupled scheme. As discussed in the previous section, the JT-coupled scheme is best suited for a many-body calculation, while the Jacobi basis is more appropriate for methods involving small particle numbers, e.g., the SRG transformation of the interaction. Therefore a transformation between the Jacobi basis and the JT-coupled scheme is necessary. The transformation is similar to the three-body case, see Ref. [13].

The isospin part is not changed by the transformation and therefore we omit it in this derivation. However, the isospin labels change to fit the naming schemes of the different bases:

$$\left|\left[\left(T_{ab}\,\tfrac{1}{2}\right)T_{abc}\,\tfrac{1}{2}\right]TM_T\right\rangle = \sum_{T_1,T_{12}}\sum_{T_{123},M_{T_{123}}} \delta_{T_1,T_{ab}}\delta_{T_{12},T_{abc}}\delta_{T_{123},T}\delta_{M_{T_{123}},M_T}\left|\left[\left(T_1\,\tfrac{1}{2}\right)T_{12}\,\tfrac{1}{2}\right]T_{123}M_{T_{123}}\right\rangle. \tag{4.21}$$

For the basis transformation multiple coordinate transformations are needed. All of them can be represented by the transformation matrix given in Eq. (3.28).

$$M_d = \begin{pmatrix} \sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}} \\ \sqrt{\frac{1}{1+d}} & -\sqrt{\frac{d}{1+d}} \end{pmatrix}, \tag{4.22}$$

where d can be deduced from the coordinates involved. The following three transformations are needed to transform the four-body coordinate system from Jacobi to particle coordinates.

$$\begin{aligned} \left(\vec{\xi}_0^{\,ab}, \vec{\xi}_1\right)^T &= M_1 \cdot \left(\vec{r}_1, \vec{r}_2\right)^T, \\ \left(\vec{\xi}_0^{\,abc}, \vec{\xi}_2\right)^T &= M_2 \cdot \left(\vec{\xi}_0^{\,ab}, \vec{r}_3\right)^T, \\ \left(\vec{\xi}_0, \vec{\xi}_3\right)^T &= M_3 \cdot \left(\vec{\xi}_0^{\,abc}, \vec{r}_4\right)^T, \end{aligned}$$

where we introduced two intermediate coordinates given by:

$$\vec{\xi}_0^{\,ab} = \sqrt{\tfrac{1}{2}}(\vec{r}_1 + \vec{r}_2), \qquad \vec{\xi}_0^{\,abc} = \sqrt{\tfrac{1}{3}}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3),$$

which are the zeroth Jacobi coordinate, i.e., the center-of-mass part, in the two- and three-body case, respectively. Note that there are other possible choices for the coordinate transformations that also connect Jacobi to particle coordinates. Starting from the JT-coupled scheme,

$$\left|n_a n_b n_c n_d; \left(\left\{\left[\left(l_a\,\tfrac{1}{2}\right)j_a\left(l_b\,\tfrac{1}{2}\right)j_b\right]J_{ab}\left(l_c\,\tfrac{1}{2}\right)j_c\right\}J_{abc}\left(l_d\,\tfrac{1}{2}\right)j_d\right)JM_J\right\rangle, \tag{4.23}$$

we will transform it to the Jacobi basis step by step, where each change is marked red for clarity. To use the coordinate transformations mentioned, we need to get a state where the relevant orbital angular momenta are coupled. For the first coordinate transformation l_a and l_b need to be coupled, which can easily be achieved using a 9-J symbol (see Eq. 3.18), yielding

$$= \sum_{L_{ab},S_1} \hat{j}_a\hat{j}_b\hat{L}_{ab}\hat{S}_{ab} \begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \left|n_a n_b n_c n_d; \left(\left\{\left[\left(l_a l_b\right)L_{ab}S_1\right]J_{ab}\left(l_c\,\tfrac{1}{2}\right)j_c\right\}J_{abc}\left(l_d\,\tfrac{1}{2}\right)j_d\right)JM_J\right\rangle. \tag{4.24}$$

This enables us to apply the first coordinate transformation,

$$= \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \hat{j}_a \hat{j}_b \hat{L}_{ab} \hat{S}_{ab} \ll N_{cm}^{ab} L_{cm}^{ab}, N_1 L_1 | n_a l_a, n_b l_b; L_{ab} \gg_1 \begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix}$$
$$\left| N_{cm}^{ab} N_1 n_c n_d; \left(\left\{ \left[\left(L_{cm}^{ab} L_1 \right) L_{ab} S_1 \right] J_{ab} \left(l_c \tfrac{1}{2} \right) j_c \right\} J_{abc} \left(l_d \tfrac{1}{2} \right) j_d \right) J M_J \right\rangle , \tag{4.25}$$

where the quantum numbers N_{cm}^{ab} and L_{cm}^{ab}, correspond to the intermediate coordinate $\vec{\xi}_0^{ab}$. For the second coordinate transformation L_{cm}^{ab} and l_c need to be coupled, which can be achieved with two transformations, involving a 6-J (see Eq. 3.12) and a 9-J symbol (see Eq. 3.18):

$$= \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \sum_{J_1} \hat{j}_a \hat{j}_b \hat{L}_{ab}^2 \hat{S}_{ab} \hat{J}_1 (-1)^{L_{cm}^{ab}+L_1+S_1+J_{ab}} \ll N_{cm}^{ab} L_{cm}^{ab}, N_1 L_1 | n_a l_a, n_b l_b; L_{ab} \gg_1$$
$$\begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix} \left| N_{cm}^{ab} N_1 n_c n_d; \left(\left\{ \left[L_{cm}^{ab} \left(L_1 S_1 \right) J_1 \right] J_{ab} \left(l_c \tfrac{1}{2} \right) j_c \right\} J_{abc} \left(l_d \tfrac{1}{2} \right) j_d \right) J M_J \right\rangle$$
$$= \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \sum_{J_1} \sum_{K,P} \hat{j}_a \hat{j}_b \hat{j}_c \hat{L}_{ab}^2 \hat{S}_{ab} \hat{J}_{ab} \hat{J}_1 \hat{K} \hat{P} (-1)^{L_{cm}^{ab}+L_1+S_1+J_{ab}} \ll N_{cm}^{ab} L_{cm}^{ab}, N_1 L_1 | n_a l_a, n_b l_b; L_{ab} \gg_1$$
$$\begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & J_1 & J_{ab} \\ l_c & \frac{1}{2} & j_c \\ K & P & J_{abc} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix}$$
$$\left| N_{cm}^{ab} n_c N_1 n_d; \left(\left\{ \left(L_{cm}^{ab} l_c \right) K \left[\left(L_1 S_1 \right) J_1 \tfrac{1}{2} \right] P \right\} J_{abc} \left(l_d \tfrac{1}{2} \right) j_d \right) J M_J \right\rangle . \tag{4.26}$$

We apply the second coordinate transformation where the quantum numbers N_{cm}^{abc} and L_{cm}^{abc} correspond to the intermediate coordinate $\vec{\xi}_0^{abc}$.

$$= \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \sum_{J_1} \sum_{K,P} \sum_{N_{cm}^{abc},L_{cm}^{abc}} \sum_{N_2,L_2} \hat{j}_a \hat{j}_b \hat{j}_c \hat{L}_{ab}^2 \hat{S}_{ab} \hat{J}_{ab} \hat{J}_1 \hat{K} \hat{P} (-1)^{L_{cm}^{ab}+L_1+S_1+J_{ab}} \ll N_{cm}^{ab} L_{cm}^{ab}, N_1 L_1 | n_a l_a, n_b l_b; L_{ab} \gg_1$$
$$\ll N_{cm}^{abc} L_{cm}^{abc}, N_2 L_2 | N_{cm}^{ab} L_{cm}^{ab}, n_c l_c; K \gg_2 \begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & J_1 & J_{ab} \\ l_c & \frac{1}{2} & j_c \\ K & P & J_{abc} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix}$$
$$\left| N_{cm}^{abc} N_2 N_1 n_d; \left(\left\{ \left(L_{cm}^{abc} L_2 \right) K \left[\left(L_1 S_1 \right) J_1 \tfrac{1}{2} \right] P \right\} J_{abc} \left(l_d \tfrac{1}{2} \right) j_d \right) J M_J \right\rangle . \tag{4.27}$$

For the final coordinate transformation L_{cm}^{abc} and l_d need to be coupled, which can be done with three additional changes to the coupling scheme.

$$= \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \sum_{J_1} \sum_{K,P} \sum_{N_{cm}^{abc},L_{cm}^{abc}} \sum_{N_2,L_2} \sum_{J_{12}} \hat{j}_a \hat{j}_b \hat{j}_c \hat{L}_{ab}^2 \hat{S}_{ab} \hat{J}_{ab} \hat{J}_1 \hat{K}^2 \hat{P} \hat{J}_{12} (-1)^{L_{cm}^{ab}+L_{cm}^{abc}+L_1+L_2+S_1+J_{ab}+J_{abc}+P}$$
$$\ll N_{cm}^{ab} L_{cm}^{ab}, N_1 L_1 | n_a l_a, n_b l_b; L_{ab} \gg_1 \ll N_{cm}^{abc} L_{cm}^{abc}, N_2 L_2 | N_{cm}^{ab} L_{cm}^{ab}, n_c l_c; K \gg_2$$
$$\begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & J_1 & J_{ab} \\ l_c & \frac{1}{2} & j_c \\ K & P & J_{abc} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & L_2 & K \\ P & J_{abc} & J_{12} \end{Bmatrix}$$
$$\left| N_{cm}^{abc} N_2 N_1 n_d; \left(\left\{ L_{cm}^{abc} \left(L_2 \left[\left(L_1 S_1 \right) J_1 \tfrac{1}{2} \right] P \right) J_{12} \right\} J_{abc} \left(l_d \tfrac{1}{2} \right) j_d \right) J M_J \right\rangle$$

$$
\begin{aligned}
&= \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \sum_{J_1} \sum_{K,P} \sum_{N_{cm}^{abc},L_{cm}^{abc}} \sum_{N_2,L_2} \sum_{J_{12}} \sum_{J_2} \hat{j}_a \hat{j}_b \hat{j}_c \hat{L}_{ab}^2 \hat{S}_{ab} \hat{J}_{ab} \hat{J}_1 \hat{K}^2 \hat{P}^2 \hat{J}_{12} \hat{J}_2 (-1)^{1+L_{cm}^{ab}+L_{cm}^{abc}+L_1+S_1+J_{ab}+J_{abc}+J_{12}} \\
&\ll N_{cm}^{ab} L_{cm}^{ab}, N_1 L_1 | n_a l_a, n_b l_b; L_{ab} \gg_1 \ll N_{cm}^{abc} L_{cm}^{abc}, N_2 L_2 | N_{cm}^{ab} L_{cm}^{ab}, n_c l_c; K \gg_2 \\
&\begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & J_1 & J_{ab} \\ l_c & \frac{1}{2} & j_c \\ K & P & J_{abc} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & L_2 & K \\ P & J_{abc} & J_{12} \end{Bmatrix} \begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ J_1 & J_{12} & P \end{Bmatrix} \\
&\left| N_{cm}^{abc} N_2 N_1 n_d; \left(\left\{ L_{cm}^{abc} \left[\left(L_2 \tfrac{1}{2} \right) J_2 \left(L_1 S_1 \right) J_1 \right] J_{12} \right\} J_{abc} \left(l_d \tfrac{1}{2} \right) j_d \right) J M_J \right\rangle \\
&= \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \sum_{J_1} \sum_{K,P} \sum_{N_{cm}^{abc},L_{cm}^{abc}} \sum_{N_2,L_2} \sum_{J_{12}} \sum_{J_2} \sum_{Q,R} \hat{j}_a \hat{j}_b \hat{j}_c \hat{j}_d \hat{L}_{ab}^2 \hat{S}_{ab} \hat{J}_{ab} \hat{J}_{abc} \hat{J}_1 \hat{K}^2 \hat{P}^2 \hat{J}_{12} \hat{J}_2 \hat{Q} \hat{R} \\
&(-1)^{1+L_{cm}^{ab}+L_{cm}^{abc}+L_1+S_1+J_{ab}+J_{abc}+J_{12}} \ll N_{cm}^{ab} L_{cm}^{ab}, N_1 L_1 | n_a l_a, n_b l_b; L_{ab} \gg_1 \ll N_{cm}^{abc} L_{cm}^{abc}, N_2 L_2 | N_{cm}^{ab} L_{cm}^{ab}, n_c l_c; K \gg_2 \\
&\begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & J_1 & J_{ab} \\ l_c & \frac{1}{2} & j_c \\ K & P & J_{abc} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & J_{12} & J_{abc} \\ l_d & \frac{1}{2} & j_d \\ Q & R & J \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & L_2 & K \\ P & J_{abc} & J_{12} \end{Bmatrix} \begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ J_1 & J_{12} & P \end{Bmatrix} \\
&\left| N_{cm}^{abc} n_d N_2 N_1; \left(\left(L_{cm}^{abc} l_d \right) Q \left\{ \left[\left(L_2 \tfrac{1}{2} \right) J_2 \left(L_1 S_1 \right) J_1 \right] J_{12} \tfrac{1}{2} \right\} R \right) J M_J \right\rangle . \qquad (4.28)
\end{aligned}
$$

With the last coordinate transformation we get the quantum numbers for the total center-of-mass:

$$
\begin{aligned}
&= \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \sum_{J_1} \sum_{K,P} \sum_{N_{cm}^{abc},L_{cm}^{abc}} \sum_{N_2,L_2} \sum_{J_{12}} \sum_{J_2} \sum_{Q,R} \sum_{N_{cm},L_{cm}} \sum_{N_3,L_3} \hat{j}_a \hat{j}_b \hat{j}_c \hat{j}_d \hat{L}_{ab}^2 \hat{S}_{ab} \hat{J}_{ab} \hat{J}_{abc} \hat{J}_1 \hat{K}^2 \hat{P}^2 \hat{J}_{12} \hat{J}_2 \hat{Q} \hat{R} \\
&(-1)^{1+L_{cm}^{ab}+L_{cm}^{abc}+L_1+S_1+J_{ab}+J_{abc}+J_{12}} \ll N_{cm}^{ab} L_{cm}^{ab}, N_1 L_1 | n_a l_a, n_b l_b; L_{ab} \gg_1 \ll N_{cm}^{abc} L_{cm}^{abc}, N_2 L_2 | N_{cm}^{ab} L_{cm}^{ab}, n_c l_c; K \gg_2 \\
&\ll N_{cm} L_{cm}, N_3 L_3 | N_{cm}^{abc} L_{cm}^{abc}, n_d l_d; Q \gg_3 \\
&\begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & J_1 & J_{ab} \\ l_c & \frac{1}{2} & j_c \\ K & P & J_{abc} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & J_{12} & J_{abc} \\ l_d & \frac{1}{2} & j_d \\ Q & R & J \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & L_2 & K \\ P & J_{abc} & J_{12} \end{Bmatrix} \begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ J_1 & J_{12} & P \end{Bmatrix} \\
&\left| N_{cm} N_3 N_2 N_1; \left(\left(L_{cm} L_3 \right) Q \left\{ \left[\left(L_2 \tfrac{1}{2} \right) J_2 \left(L_1 S_1 \right) J_1 \right] J_{12} \tfrac{1}{2} \right\} R \right) J M_J \right\rangle . \\
&= \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \sum_{J_1} \sum_{K,P} \sum_{N_{cm}^{abc},L_{cm}^{abc}} \sum_{N_2,L_2} \sum_{J_{12}} \sum_{J_2} \sum_{Q,R} \sum_{N_{cm},L_{cm}} \sum_{N_3,L_3} \sum_{J_{123}} \hat{j}_a \hat{j}_b \hat{j}_c \hat{j}_d \hat{L}_{ab}^2 \hat{S}_{ab} \hat{J}_{ab} \hat{J}_{abc} \hat{J}_1 \hat{K}^2 \hat{P}^2 \hat{J}_{12} \hat{J}_2 \hat{Q}^2 \hat{R} \hat{J}_{123} \\
&(-1)^{1+L_{cm}^{ab}+L_{cm}^{abc}+L_{cm}+L_1+L_3+S_1+J_{ab}+J_{abc}+J_{12}+R+J} \ll N_{cm}^{ab} L_{cm}^{ab}, N_1 L_1 | n_a l_a, n_b l_b; L_{ab} \gg_1 \\
&\ll N_{cm}^{abc} L_{cm}^{abc}, N_2 L_2 | N_{cm}^{ab} L_{cm}^{ab}, n_c l_c; K \gg_2 \ll N_{cm} L_{cm}, N_3 L_3 | N_{cm}^{abc} L_{cm}^{abc}, n_d l_d; Q \gg_3 \\
&\begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & J_1 & J_{ab} \\ l_c & \frac{1}{2} & j_c \\ K & P & J_{abc} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & J_{12} & J_{abc} \\ l_d & \frac{1}{2} & j_d \\ Q & R & J \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & L_2 & K \\ P & J_{abc} & J_{12} \end{Bmatrix} \begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ J_1 & J_{12} & P \end{Bmatrix} \\
&\begin{Bmatrix} L_{cm} & L_3 & Q \\ R & J & J_{123} \end{Bmatrix} \left| N_{cm} N_3 N_2 N_1; \left(L_{cm} \left(L_3 \left\{ \left[\left(L_2 \tfrac{1}{2} \right) J_2 \left(L_1 S_1 \right) J_1 \right] J_{12} \tfrac{1}{2} \right\} R \right) J_{123} \right) J M_J \right\rangle \\
&= \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \sum_{J_1} \sum_{K,P} \sum_{N_{cm}^{abc},L_{cm}^{abc}} \sum_{N_2,L_2} \sum_{J_{12}} \sum_{J_2} \sum_{Q,R} \sum_{N_{cm},L_{cm}} \sum_{N_3,L_3} \sum_{J_{123}} \sum_{J_3} \hat{j}_a \hat{j}_b \hat{j}_c \hat{j}_d \hat{L}_{ab}^2 \hat{S}_{ab} \hat{J}_{ab} \hat{J}_{abc} \hat{J}_1 \hat{K}^2 \hat{P}^2 \hat{J}_{12} \hat{J}_2 \hat{Q}^2 \hat{R}^2 \hat{J}_{123} \hat{J}_3 \\
&(-1)^{1+L_{cm}^{ab}+L_{cm}^{abc}+L_{cm}+L_1+S_1+J_{ab}+J_{abc}+J_{12}+J_{123}+J} \ll N_{cm}^{ab} L_{cm}^{ab}, N_1 L_1 | n_a l_a, n_b l_b; L_{ab} \gg_1 \\
&\ll N_{cm}^{abc} L_{cm}^{abc}, N_2 L_2 | N_{cm}^{ab} L_{cm}^{ab}, n_c l_c; K \gg_2 \ll N_{cm} L_{cm}, N_3 L_3 | N_{cm}^{abc} L_{cm}^{abc}, n_d l_d; Q \gg_3 \\
&\begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & J_1 & J_{ab} \\ l_c & \frac{1}{2} & j_c \\ K & P & J_{abc} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & J_{12} & J_{abc} \\ l_d & \frac{1}{2} & j_d \\ Q & R & J \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & L_2 & K \\ P & J_{abc} & J_{12} \end{Bmatrix} \begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ J_1 & J_{12} & P \end{Bmatrix} \\
&\begin{Bmatrix} L_{cm} & L_3 & Q \\ R & J & J_{123} \end{Bmatrix} \begin{Bmatrix} L_3 & \frac{1}{2} & J_3 \\ J_{12} & J_{123} & R \end{Bmatrix} \left| N_{cm} N_3 N_2 N_1; \left(L_{cm} \left\{ \left(L_3 \tfrac{1}{2} \right) J_3 \left[\left(L_2 \tfrac{1}{2} \right) J_2 \left(L_1 S_1 \right) J_1 \right] J_{12} \right\} J_{123} \right) J M_J \right\rangle , \qquad (4.29)
\end{aligned}
$$

where we used two 6-J symbols to change the coupling scheme to the non-antisymmetric Jacobi basis. We now have L_{cm} coupled to J_{123}. For a separation of the center-of-mass part, we use CGCs in the following step. Furthermore, we change the coupling order in the relative part which yields a factor of $(-1)^{J_1+J_2+J_3-J_{123}}$:

$$
\begin{aligned}
&= \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \sum_{J_1} \sum_{K,P} \sum_{N_{cm}^{abc},L_{cm}^{abc}} \sum_{N_2,L_2} \sum_{J_{12}} \sum_{J_2} \sum_{Q,R} \sum_{N_{cm},L_{cm}} \sum_{N_3,L_3} \sum_{J_{123}} \sum_{J_3} \sum_{M_{L_{cm}},M_{J_{123}}} \\
&\quad \hat{j}_a\hat{j}_b\hat{j}_c\hat{j}_d\hat{L}_{ab}^2\hat{S}_{ab}\hat{J}_{ab}\hat{J}_{abc}\hat{J}_1\hat{K}^2\hat{P}^2\hat{J}_{12}\hat{J}_2\hat{Q}^2\hat{R}^2\hat{J}_{123}\hat{J}_3(-1)^{1+L_{cm}^{ab}+L_{cm}^{abc}+L_{cm}+L_1+S_1+J_{ab}+J_{abc}+J_{12}+J+J_1+J_2+J_3} \\
&\quad \ll N_{cm}^{ab}L_{cm}^{ab},N_1L_1|n_al_a,n_bl_b;L_{ab}\gg_1 \ll N_{cm}^{abc}L_{cm}^{abc},N_2L_2|N_{cm}^{ab}L_{cm}^{ab},n_cl_c;K\gg_2 \ll N_{cm}L_{cm},N_3L_3|N_{cm}^{abc}L_{cm}^{abc},n_dl_d;Q\gg_3 \\
&\quad \begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & J_1 & J_{ab} \\ l_c & \frac{1}{2} & j_c \\ K & P & J_{abc} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & J_{12} & J_{abc} \\ l_d & \frac{1}{2} & j_d \\ Q & R & J \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & L_2 & K \\ P & J_{abc} & J_{12} \end{Bmatrix} \\
&\quad \begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ J_1 & J_{12} & P \end{Bmatrix} \begin{Bmatrix} L_{cm} & L_3 & Q \\ R & J & J_{123} \end{Bmatrix} \begin{Bmatrix} L_3 & \frac{1}{2} & J_3 \\ J_{12} & J_{123} & R \end{Bmatrix} c \begin{pmatrix} L_{cm} & J_{123} & J \\ M_{L_{cm}} & M_{J_{123}} & M_J \end{pmatrix} \\
&\quad \left| N_{cm}L_{cm}M_{L_{cm}};N_1N_2N_3;\left\{\left[\left(L_1S_1\right)J_1\left(L_2\tfrac{1}{2}\right)J_2\right]J_{12}\left(L_3\tfrac{1}{2}\right)J_3\right\}J_{123}M_{J_{123}}\right\rangle .
\end{aligned}
\tag{4.30}
$$

We can now transform the non-antisymmetric Jacobi basis to the non-antisymmetric JT-coupled scheme. Using the antisymmetrizer we can obtain the same transformation for fully antisymmetric basis states. Special care must be taken regarding the introduced normalization constant. If we antisymmetrize the m-scheme an additional factor of $\sqrt{4!}$ is needed to get a normalized basis. We will use the same factor for the coupled case, this does not, however, imply that the coupled state is normalized. It is not even orthogonal. This is of no concern as the final calculation will be done in the m-scheme, decoupling the matrix elements on the fly. The factor ensures that decoupling the states yields a normalized basis. For the Jacobi basis the antisymmetrizer simply yields sums over i_{12} and i_{123} along with three-body and four-body CFPs. Furthermore, the isospin part is added again for completeness:

$$
\begin{aligned}
&\left|EJM_JTM_T\alpha_{abcd}\right\rangle_a \\
&\quad = \sqrt{4!}\mathcal{A}\left|EJM_JTM_T\alpha_{abcd}\right\rangle \\
&\quad = \sqrt{4!} \sum_{L_{ab},S_1} \sum_{N_{cm}^{ab},L_{cm}^{ab}} \sum_{N_1,L_1} \sum_{J_1} \sum_{K,P} \sum_{N_{cm}^{abc},L_{cm}^{abc}} \sum_{N_2,L_2} \sum_{J_{12}} \sum_{J_2} \sum_{Q,R} \sum_{N_{cm},L_{cm}} \sum_{N_3,L_3} \sum_{J_{123}} \sum_{J_3} \sum_{M_{L_{cm}},M_{J_{123}}} \sum_{i_{12}} \sum_{i_{123}} \sum_{T_1} \sum_{T_{12}} \sum_{T_{123},M_{T_{123}}} \\
&\qquad \hat{j}_a\hat{j}_b\hat{j}_c\hat{j}_d\hat{L}_{ab}^2\hat{S}_{ab}\hat{J}_{ab}\hat{J}_{abc}\hat{J}_1\hat{K}^2\hat{P}^2\hat{J}_{12}\hat{J}_2\hat{Q}^2\hat{R}^2\hat{J}_{123}\hat{J}_3(-1)^{1+L_{cm}^{ab}+L_{cm}^{abc}+L_{cm}+L_1+S_1+J_{ab}+J_{abc}+J_{12}+J+J_1+J_2+J_3} \\
&\qquad \ll N_{cm}^{ab}L_{cm}^{ab},N_1L_1|n_al_a,n_bl_b;L_{ab}\gg_1 \ll N_{cm}^{abc}L_{cm}^{abc},N_2L_2|N_{cm}^{ab}L_{cm}^{ab},n_cl_c;K\gg_2 \ll N_{cm}L_{cm},N_3L_3|N_{cm}^{abc}L_{cm}^{abc},n_dl_d;Q\gg_3 \\
&\qquad \begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & J_1 & J_{ab} \\ l_c & \frac{1}{2} & j_c \\ K & P & J_{abc} \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & J_{12} & J_{abc} \\ l_d & \frac{1}{2} & j_d \\ Q & R & J \end{Bmatrix} \begin{Bmatrix} L_{cm}^{ab} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix} \begin{Bmatrix} L_{cm}^{abc} & L_2 & K \\ P & J_{abc} & J_{12} \end{Bmatrix} \\
&\qquad \begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ J_1 & J_{12} & P \end{Bmatrix} \begin{Bmatrix} L_{cm} & L_3 & Q \\ R & J & J_{123} \end{Bmatrix} \begin{Bmatrix} L_3 & \frac{1}{2} & J_3 \\ J_{12} & J_{123} & R \end{Bmatrix} c \begin{pmatrix} L_{cm} & J_{123} & J \\ M_{L_{cm}} & M_{J_{123}} & M_J \end{pmatrix} \delta_{T_1,T_{ab}}\delta_{T_{12},T_{abc}}\delta_{T_{123},T}\delta_{M_{T_{123}},M_T} \\
&\qquad c_{N_1,L_1,S_1,J_1,T_1,N_2,L_2,J_2}^{E_{12},i_{12},J_{12},T_{12}} \tilde{c}_{E_{12},i_{12},J_{12},T_{12},N_3,L_3,J_3}^{E_{123},i_{123},J_{123},T_{123}} \left|N_{cm}L_{cm}M_{L_{cm}};E_{123}i_{123}J_{123}M_{J_{123}}T_{123}M_{T_{123}}\right\rangle_a ,
\end{aligned}
\tag{4.31}
$$

which will be abbreviated using a transformation coefficient $\tilde{T}$.

$$
\begin{aligned}
&= \sqrt{4!} \sum_{N_{cm},L_{cm}} \sum_{M_{L_{cm}}} \sum_{E_{123}} \sum_{J_{123}} \sum_{M_{J_{123}}} \sum_{T_{123}} \sum_{M_{T_{123}}} \sum_{i_{123}} \tilde{T}_{N_{cm},L_{cm},E,J,\alpha_{abcd}}^{E_{123},J_{123},T_{123},i_{123}} c \begin{pmatrix} L_{cm} & J_{123} & J \\ M_{L_{cm}} & M_{J_{123}} & M_J \end{pmatrix} \\
&\quad \delta_{T_{123},T}\delta_{M_{T_{123}},M_T} \left|N_{cm}L_{cm}M_{L_{cm}};E_{123}i_{123}J_{123}M_{J_{123}}T_{123}M_{T_{123}}\right\rangle_a ,
\end{aligned}
\tag{4.32}
$$

where the transformation coefficient is given by:

$$
\begin{aligned}
\tilde{T}^{E_{123},J_{123},T_{123},i_{123}}_{N_{\rm cm},L_{\rm cm},E,J,\alpha_{abcd}} = & \sum_{k_{123}} \sum_{k_{12}} \sum_{L_{ab}} \sum_{K,P} \sum_{Q,R} \sum_{N^{ab}_{cm},L^{ab}_{cm}} \sum_{N^{abc}_{cm},L^{abc}_{cm}} \delta_{T_1,T_{ab}} \delta_{T_{12},T_{abc}} \hat{j}_a \hat{j}_b \hat{j}_c \hat{j}_d \hat{L}^2_{ab} \hat{S}_{ab} \hat{J}_{ab} \hat{J}_{abc} \hat{J}_1 \hat{K}^2 \hat{P}^2 \hat{J}_{12} \hat{J}_2 \hat{Q}^2 \hat{R}^2 \hat{J}_{123} \hat{J}_3 \\
& (-1)^{1+L^{ab}_{cm}+L^{abc}_{cm}+L_{cm}+L_1+S_1+J_{ab}+J_{abc}+J_{12}+J+J_1+J_2+J_3} \ll N^{ab}_{cm} L^{ab}_{cm}, N_1 L_1 | n_a l_a, n_b l_b; L_{ab} \gg_1 \\
& \ll N^{abc}_{cm} L^{abc}_{cm}, N_2 L_2 | N^{ab}_{cm} L^{ab}_{cm}, n_c l_c; K \gg_2 \ll N_{cm} L_{cm}, N_3 L_3 | N^{abc}_{cm} L^{abc}_{cm}, n_d l_d; Q \gg_3 \\
& \begin{Bmatrix} l_a & \frac{1}{2} & j_a \\ l_b & \frac{1}{2} & j_b \\ L_{ab} & S_1 & J_{ab} \end{Bmatrix} \begin{Bmatrix} L^{ab}_{cm} & J_1 & J_{ab} \\ l_c & \frac{1}{2} & j_c \\ K & P & J_{abc} \end{Bmatrix} \begin{Bmatrix} L^{abc}_{cm} & J_{12} & J_{abc} \\ l_d & \frac{1}{2} & j_d \\ Q & R & J \end{Bmatrix} \begin{Bmatrix} L^{ab}_{cm} & L_1 & L_{ab} \\ S_1 & J_{ab} & J_1 \end{Bmatrix} \begin{Bmatrix} L^{abc}_{cm} & L_2 & K \\ P & J_{abc} & J_{12} \end{Bmatrix} \\
& \begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ J_1 & J_{12} & P \end{Bmatrix} \begin{Bmatrix} L_{cm} & L_3 & Q \\ R & J & J_{123} \end{Bmatrix} \begin{Bmatrix} L_3 & \frac{1}{2} & J_3 \\ J_{12} & J_{123} & R \end{Bmatrix} c^{E_{12},i_{12},J_{12},T_{12}}_{k_{12}} \tilde{c}^{E_{123},i_{123},J_{123},T_{123}}_{k_{123}}.
\end{aligned} \tag{4.33}
$$

The sums over N_1, L_1, S_1, J_1, T_1, N_2, L_2 and J_2 have been combined using a sum over E_{12} and k_{12} (see Sec. 4.1.3) and the sums over E_{12}, J_{12}, T_{12}, i_{12}, N_3, L_3 and J_3 have been combined using a sum over E_{123} and k_{123} (see Sec. 4.1.4). We now have a look at the transformation of the matrix elements, which is easily constructed using the derived expression:

$$
\begin{aligned}
& {}_a\left\langle E'J'M'_J T'M'_T \alpha'_{abcd} \right| V_{4N} \left| EJM_J TM_T \alpha_{abcd} \right\rangle_a \\
& \quad = 4! \sum_{N_{cm},L_{cm}} \sum_{M_{L_{cm}}} \sum_{E_{123}} \sum_{J_{123}} \sum_{M_{J_{123}}} \sum_{T_{123}} \sum_{M_{T_{123}}} \sum_{i_{123}} \sum_{N'_{cm},L'_{cm}} \sum_{M'_{L_{cm}}} \sum_{E'_{123}} \sum_{J'_{123}} \sum_{M'_{J_{123}}} \sum_{T'_{123}} \sum_{M'_{T_{123}}} \sum_{i'_{123}} \\
& \quad \tilde{T}^{E_{123},J_{123},T_{123},i_{123}}_{N_{\rm cm},L_{\rm cm},E,J,\alpha_{abcd}} \tilde{T}^{E'_{123},J'_{123},T'_{123},i'_{123}}_{N'_{\rm cm},L'_{\rm cm},E',J',\alpha'_{abcd}} \mathrm{c} \begin{pmatrix} L_{cm} & J_{123} & J \\ M_{L_{cm}} & M_{J_{123}} & M_J \end{pmatrix} \mathrm{c} \begin{pmatrix} L'_{cm} & J'_{123} & J' \\ M'_{L_{cm}} & M'_{J_{123}} & M'_J \end{pmatrix} \\
& \quad \delta_{T_{123},T} \delta_{M_{T_{123}},M_T} \delta_{T'_{123},T'} \delta_{M'_{T_{123}},M'_T} \\
& \quad {}_a\left\langle N'_{cm} L'_{cm} M'_{L_{cm}}; E'_{123} i'_{123} J'_{123} M'_{J_{123}} T'_{123} M'_{T_{123}} \right| V_{4N} \left| N_{cm} L_{cm} M_{L_{cm}}; E_{123} i_{123} J_{123} M_{J_{123}} T_{123} M_{T_{123}} \right\rangle_a,
\end{aligned} \tag{4.34}
$$

which can be simplified by using the following properties of our interaction, which have been discussed in Sec. 4.3:

- The interaction is independent of the center-of-mass part.
- The interaction is diagonal in isospin, i.e., T_{123} and $M_{T_{123}}$.
- The interaction is diagonal in angular momentum, i.e., J_{123} and $M_{J_{123}}$.
- The interaction is independent of the two projection quantum numbers $M_{J_{123}}$ and $M_{T_{123}}$.

This yields the following δ-functions: $\delta_{N_{cm},N'_{cm}}$, $\delta_{L_{cm},L'_{cm}}$, $\delta_{M_{L_{cm}},M'_{L_{cm}}}$, $\delta_{T_{123},T'_{123}}$, $\delta_{M_{T_{123}},M'_{T_{123}}}$, $\delta_{J_{123},J'_{123}}$ and $\delta_{M_{J_{123}},M'_{J_{123}}}$. Using these functions and the orthogonality relation of the Clebsch-Gordan coefficients (Eq. 3.7) we can carry out the sum over $M_{L_{cm}}$ and $M_{J_{123}}$ which yields two additional δ functions: $\delta_{J,J'}$ and δ_{M_J,M'_J}. These make the resulting interaction matrix elements diagonal in angular momentum and independent of M_J and M_T:

$$
\begin{aligned}
& {}_a\left\langle E'J'M'_J T'M'_T \alpha'_{abcd} \right| V_{4N} \left| EJM_J TM_T \alpha_{abcd} \right\rangle_a \\
& \quad = 4! \, \delta_{J,J'} \delta_{M_J,M'_J} \delta_{T,T'} \delta_{M_T,M'_T} \sum_{N_{cm},L_{cm}} \sum_{E_{123}} \sum_{J_{123}} \sum_{T_{123}} \sum_{i_{123}} \sum_{E'_{123}} \sum_{i'_{123}} \\
& \quad \tilde{T}^{E_{123},J_{123},T_{123},i_{123}}_{N_{\rm cm},L_{\rm cm},E,J,\alpha_{abcd}} \; \tilde{T}^{E'_{123},J_{123},T_{123},i'_{123}}_{N_{\rm cm},L_{\rm cm},E',J,\alpha'_{abcd}} \; \delta_{T_{123},T} \; {}_a\left\langle E'_{123} i'_{123} J_{123} T_{123} \right| V_{4N} \left| E_{123} i_{123} J_{123} T_{123} \right\rangle_a.
\end{aligned} \tag{4.35}
$$

The transformation allows to include the four-body forces in a many-body calculation in an exact manner. The only restriction in this case is the truncation of the four-body model space using the JT-coupled scheme, as discussed in Sec. 4.3.

4.5 Reduction to Effective Three-Body Interaction

We have derived a transformation from the four-body Jacobi basis to the JT-coupled scheme, which allows us to incorporate the four-body forces in a many-body calculation. However, using four-body forces in a many-body method requires more computation time than using three-body forces only. More importantly, most many-body methods cannot handle four-body forces. We, therefore, devise a method to reduce the matrix elements from the four-body Jacobi basis to the three-body Jacobi basis. This transformation is devised to be simple and provide a fast check of the effect of the four-body forces. As it involves a sum over the quantum numbers of one particle, we name it partial-trace approximation. Keep in mind that this is an uncontrolled approximation.

The first step necessary is the transformation from the four-body Jacobi basis to the following basis:

$$\left\{ \left| N_{cm}^{abc} L_{cm}^{abc} M_{L_{cm}^{abc}} \right\rangle \left| E_{12} i_{12} J_{12} M_{J_{12}} T_{12} M_{T_{12}} \right\rangle_a \left| n_d l_d ; j_d m_{j_d} ; \tfrac{1}{2} m_{t_d} \right\rangle \right\}_a , \tag{4.36}$$

which is a combination of the antisymmetric three-body Jacobi basis and a single-particle HO basis for the fourth particle.

We start by explicitly antisymmetrizing the state, but to do that, we need to determine the factor that is introduced by using the antisymmetrization operator. If we apply it on a non antisymmetric four-body product state of single-particle states we obtain a factor of $\sqrt{4!}$:

$$\mathcal{A} \left| abcd \right\rangle = \tfrac{1}{\sqrt{4!}} \left| abcd \right\rangle_a \tag{4.37}$$

A three-body antisymmetrizer $\mathcal{A}_{123}$ yields a factor of $\sqrt{3!}$ only:

$$\left(\mathcal{A}_{123} \left| abc \right\rangle \right) \left| d \right\rangle = \tfrac{1}{\sqrt{3!}} \left| abc \right\rangle_a \left| d \right\rangle \tag{4.38}$$

Applying the complete antisymmetrizer $\mathcal{A}$ on the state from Eq. (4.38) should yield the same result as before:

$$\mathcal{A} \tfrac{1}{\sqrt{3!}} \left| abc \right\rangle_a \left| d \right\rangle = \tfrac{1}{\sqrt{4!}} \left| abcd \right\rangle_a \Rightarrow \left| abcd \right\rangle_a = \sqrt{4} \mathcal{A} \left| abc \right\rangle_a \left| d \right\rangle . \tag{4.39}$$

Since the state from Eq. (4.36) is antisymmetric under permutation of the first three particles, we are left with a factor of $\sqrt{4}$. Furthermore we need to couple the orbital angular momentum of the fourth particle to the three-body center-of-mass orbital angular momentum. This is done using two CGCs, where the changes are marked red:

$$\left\{ \left| N_{cm}^{abc} L_{cm}^{abc} M_{L_{cm}^{abc}} \right\rangle \left| E_{12} i_{12} J_{12} M_{J_{12}} T_{12} M_{T_{12}} \right\rangle_a \left| n_d l_d ; j_d m_{j_d} ; \tfrac{1}{2} m_{t_d} \right\rangle \right\}_a \tag{4.40}$$

$$= \sqrt{4} \mathcal{A} \left| N_{cm}^{abc} L_{cm}^{abc} M_{L_{cm}^{abc}} \right\rangle \left| E_{12} i_{12} J_{12} M_{J_{12}} T_{12} M_{T_{12}} \right\rangle_a \left| n_d l_d ; j_d m_{j_d} ; \tfrac{1}{2} m_{t_d} \right\rangle \tag{4.41}$$

$$= \sqrt{4} \mathcal{A} \sum_{m_{l_d} m_{s_d}} \mathrm{c} \begin{pmatrix} l_d & \frac{1}{2} & j_d \\ m_{l_d} & m_{s_d} & m_{j_d} \end{pmatrix} \left| N_{cm}^{abc} L_{cm}^{abc} M_{L_{cm}^{abc}} \right\rangle \left| E_{12} i_{12} J_{12} M_{J_{12}} T_{12} M_{T_{12}} \right\rangle_a \left| n_d l_d m_{l_d} ; \tfrac{1}{2} m_{s_d} ; \tfrac{1}{2} m_{t_d} \right\rangle \tag{4.42}$$

$$= \sqrt{4} \mathcal{A} \sum_{m_{l_d} m_{s_d}} \sum_{K, M_K} \mathrm{c} \begin{pmatrix} l_d & \frac{1}{2} & j_d \\ m_{l_d} & m_{s_d} & m_{j_d} \end{pmatrix} \mathrm{c} \begin{pmatrix} L_{cm}^{abc} & l_d & K \\ M_{L_{cm}^{abc}} & m_{l_d} & M_K \end{pmatrix} \left| \left(N_{cm}^{abc} L_{cm}^{abc} n_d l_d \right) K M_K \right\rangle \left| E_{12} i_{12} J_{12} M_{J_{12}} T_{12} M_{T_{12}} \right\rangle_a \left| \tfrac{1}{2} m_{s_d} ; \tfrac{1}{2} m_{t_d} \right\rangle . \tag{4.43}$$

We continue with a coordinate transformation, where we transform the coordinates $\xi_0^{abc} = \sqrt{\frac{1}{3}} \left(r_1 + r_2 + r_3 \right)$ and r_4 to the four-body Jacobi coordinates, using the following transformation:

$$\begin{pmatrix} \xi_0 \\ \xi_3 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{\sqrt{3}}{2} \end{pmatrix} \begin{pmatrix} \xi_0^{abc} \\ r_4 \end{pmatrix} , \tag{4.44}$$

which is the transformation matrix defined in Eq. (3.28) with $d = 3$. Applying Eqs. (3.29) and (3.30) we can express the coordinate transformation with an HOB:

$$\sqrt{4} \mathcal{A} \left| N_{cm}^{abc} L_{cm}^{abc} M_{L_{cm}^{abc}} \right\rangle \left| E_{12} i_{12} J_{12} M_{J_{12}} T_{12} M_{T_{12}} \right\rangle_a \left| n_d l_d ; j_d m_{j_d} ; \tfrac{1}{2} m_{t_d} \right\rangle \tag{4.45}$$

$$= \sqrt{4} \mathcal{A} \sum_{m_{l_d} m_{s_d}} \sum_{K, M_K} \sum_{N_{cm}, L_{cm}, N_3, L_3} \mathrm{c} \begin{pmatrix} l_d & \frac{1}{2} & j_d \\ m_{l_d} & m_{s_d} & m_{j_d} \end{pmatrix} \mathrm{c} \begin{pmatrix} L_{cm}^{abc} & l_d & K \\ M_{L_{cm}^{abc}} & m_{l_d} & M_K \end{pmatrix} \ll N_{cm} L_{cm}, N_3 L_3 | N_{cm}^{abc} L_{cm}^{abc}, n_d l_d ; K \gg_3$$

$$\left| \left(N_{cm} L_{cm} N_3 L_3 \right) K M_K \right\rangle \left| E_{12} i_{12} J_{12} M_{J_{12}} T_{12} M_{T_{12}} \right\rangle_a \left| \tfrac{1}{2} m_{s_d} ; \tfrac{1}{2} m_{t_d} \right\rangle . \tag{4.46}$$

Clebsch-Gordan coefficients are used to change the coupling:

$$
\begin{aligned}
=&\sqrt{4}\mathcal{A}\sum_{m_{l_d}m_{s_d}}\sum_{K,M_K}\sum_{N_{cm},L_{cm},N_3,L_3}\sum_{M_{L_{cm}},M_{L_3}} \mathrm{c}\begin{pmatrix} l_d & \frac{1}{2} & j_d \\ m_{l_d} & m_{s_d} & m_{j_d}\end{pmatrix}\mathrm{c}\begin{pmatrix} L_{cm}^{abc} & l_d & K \\ M_{L_{cm}^{abc}} & m_{l_d} & M_K\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} L_{cm} & L_3 & K \\ M_{L_{cm}} & M_{L_3} & M_K\end{pmatrix} \ll N_{cm}L_{cm},N_3L_3|N_{cm}^{abc}L_{cm}^{abc},n_dl_d;K\gg_3\\
&\left|N_{cm}L_{cm}M_{L_{cm}}\right\rangle\left|E_{12}i_{12}J_{12}M_{J_{12}}T_{12}M_{T_{12}}\right\rangle_a\left|N_3L_3M_{L_3}\right\rangle\left|\tfrac{1}{2}m_{s_d};\tfrac{1}{2}m_{t_d}\right\rangle
\end{aligned}
\tag{4.47}
$$

$$
\begin{aligned}
=&\sqrt{4}\mathcal{A}\sum_{m_{l_d}m_{s_d}}\sum_{K,M_K}\sum_{N_{cm},L_{cm},N_3,L_3}\sum_{M_{L_{cm}},M_{L_3}}\sum_{J_3,M_{J_3}} \mathrm{c}\begin{pmatrix} l_d & \frac{1}{2} & j_d \\ m_{l_d} & m_{s_d} & m_{j_d}\end{pmatrix}\mathrm{c}\begin{pmatrix} L_{cm}^{abc} & l_d & K \\ M_{L_{cm}^{abc}} & m_{l_d} & M_K\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} L_{cm} & L_3 & K \\ M_{L_{cm}} & M_{L_3} & M_K\end{pmatrix}\mathrm{c}\begin{pmatrix} L_3 & \frac{1}{2} & J_3 \\ M_{L_3} & m_{s_d} & M_{J_3}\end{pmatrix} \ll N_{cm}L_{cm},N_3L_3|N_{cm}^{abc}L_{cm}^{abc},n_dl_d;K\gg_3\\
&\left|N_{cm}L_{cm}M_{L_{cm}}\right\rangle\left|E_{12}i_{12}J_{12}M_{J_{12}}T_{12}M_{T_{12}}\right\rangle_a\left|N_3;\left(L_3\tfrac{1}{2}\right)J_3M_{J_3};\tfrac{1}{2}m_{t_d}\right\rangle.
\end{aligned}
\tag{4.48}
$$

We finally couple J_3 with J_{12} and the isospin of the fourth particle with T_{12}, yielding the partially antisymmetric four-body Jacobi basis $\left|N_{cm}L_{cm}M_{L_{cm}}\right\rangle\left|E_{123}J_{123}M_{J_{123}}T_{123}M_{T_{123}}k_{123}\right\rangle$

$$
\begin{aligned}
:=&\sqrt{4}\mathcal{A}\sum_{m_{l_d}m_{s_d}}\sum_{K,M_K}\sum_{N_{cm},L_{cm},N_3,L_3}\sum_{M_{L_{cm}},M_{L_3}}\sum_{J_3,M_{J_3}}\sum_{J_{123},M_{J_{123}}}\sum_{T_{123},M_{T_{123}}} \mathrm{c}\begin{pmatrix} l_d & \frac{1}{2} & j_d \\ m_{l_d} & m_{s_d} & m_{j_d}\end{pmatrix}\mathrm{c}\begin{pmatrix} L_{cm}^{abc} & l_d & K \\ M_{L_{cm}^{abc}} & m_{l_d} & M_K\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} L_{cm} & L_3 & K \\ M_{L_{cm}} & M_{L_3} & M_K\end{pmatrix}\mathrm{c}\begin{pmatrix} L_3 & \frac{1}{2} & J_3 \\ M_{L_3} & m_{s_d} & M_{J_3}\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{12} & J_3 & J_{123} \\ M_{J_{12}} & M_{J_3} & M_{J_{123}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{12} & \frac{1}{2} & T_{123} \\ M_{T_{12}} & m_{t_d} & M_{T_{123}}\end{pmatrix}\\
&\ll N_{cm}L_{cm},N_3L_3|N_{cm}^{abc}L_{cm}^{abc},n_dl_d;K\gg_3\left|N_{cm}L_{cm}M_{L_{cm}}\right\rangle\left|E_{123}J_{123}M_{J_{123}}T_{123}M_{T_{123}}k_{123}\right\rangle,
\end{aligned}
\tag{4.49}
$$

where k_{123} is a shorthand for the remaining quantum numbers (see Sec. 4.1.4). The antisymmetrizer can now be applied again, which yields the CFP $\tilde{c}_{k_{123}}^{E_{123},J_{123},T_{123},i_{123}}$.

$$
\begin{aligned}
=&\sqrt{4}\sum_{m_{l_d}m_{s_d}}\sum_{K,M_K}\sum_{N_{cm},L_{cm},N_3,L_3}\sum_{M_{L_{cm}},M_{L_3}}\sum_{J_3,M_{J_3}}\sum_{J_{123},M_{J_{123}}}\sum_{T_{123},M_{T_{123}}}\sum_{i_{123}} \mathrm{c}\begin{pmatrix} l_d & \frac{1}{2} & j_d \\ m_{l_d} & m_{s_d} & m_{j_d}\end{pmatrix}\mathrm{c}\begin{pmatrix} L_{cm}^{abc} & l_d & K \\ M_{L_{cm}^{abc}} & m_{l_d} & M_K\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} L_{cm} & L_3 & K \\ M_{L_{cm}} & M_{L_3} & M_K\end{pmatrix}\mathrm{c}\begin{pmatrix} L_3 & \frac{1}{2} & J_3 \\ M_{L_3} & m_{s_d} & M_{J_3}\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{12} & J_3 & J_{123} \\ M_{J_{12}} & M_{J_3} & M_{J_{123}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{12} & \frac{1}{2} & T_{123} \\ M_{T_{12}} & m_{t_d} & M_{T_{123}}\end{pmatrix}\\
&\ll N_{cm}L_{cm},N_3L_3|N_{cm}^{abc}L_{cm}^{abc},n_dl_d;K\gg_3\tilde{c}_{k_{123}}^{E_{123},J_{123},T_{123},i_{123}}\left|N_{cm}L_{cm}M_{L_{cm}}\right\rangle\left|E_{123}i_{123}J_{123}M_{J_{123}}T_{123}M_{T_{123}}\right\rangle_a.
\end{aligned}
\tag{4.50}
$$

We now reduce the four-body matrix elements to three-body matrix elements by summing over the quantum number of the fourth particle. For the sum we omit all matrix elements that are not diagonal in the quantum numbers of the foruth particle. Additionally, the sum needs to be finite and we limit it to states that are occupied in an unperturbed Slater determinant of single-particle HO states. For closed-shell nuclei this is easily done, as only one possible Slater determinant exists for such nuclei. For open-shell nuclei we have to take multiple configurations into account. As this would require additional complexity and this method should be a simple test of the effect of four-body forces, we will focus on closed-shell nuclei.

For obtaining an effective three-body interaction that has the same properties as an initial three-body interaction, we need some additional approximations. The interaction should be independent of the three-body center-of-mass. We enforce this by ignoring center-of-mass effects and setting all associated quantum numbers to the ground state ($N_{cm}^{abc} = L_{cm}^{abc} = M_{L_{cm}^{abc}} = 0$). Furthermore, the effective three-body interaction should be diagonal in angular momentum and isospin. This does not require any approximation if we investigate closed shell nuclei with the same number of protons and neutrons. In all other cases, we achieve this requirement by simply omitting all

non-diagonal matrix elements. Finally, we also want the effective three-body interaction to be independent of the projection quantum numbers and therefore we average over $M_{J_{12}}$ and $M_{T_{12}}$.

$$
\begin{aligned}
&{}_a\left\langle E'_{12}, i'_{12}, J_{12}, T_{12}\right| V_{3N}^{eff} \left|E_{12}, i_{12}, J_{12}, T_{12}\right\rangle_a \\
&= \hat{J}_{12}^{-2}\hat{T}_{12}^{-2} \sum_{M_{J_{12}}} \sum_{M_{T_{12}}} \sum_{n_d,l_d,j_d,m_{j_d},m_{t_d}} \\
&\quad {}_a\left\{\left\langle 000\right| {}_a\left\langle E'_{12} i'_{12} J_{12} M_{J_{12}} T_{12} M_{T_{12}}\right| \left\langle n_d l_d; j_d m_{j_d}; \tfrac{1}{2} m_{t_d}\right|\right\} V_{4N} \left\{\left|000\right\rangle \left|E_{12} i_{12} J_{12} M_{J_{12}} T_{12} M_{T_{12}}\right\rangle_a \left|n_d l_d; j_d m_{j_d}; \tfrac{1}{2} m_{t_d}\right\rangle\right\}_a \\
&= 4\, \hat{J}_{12}^{-2}\hat{T}_{12}^{-2} \sum_{M_{J_{12}}} \sum_{M_{T_{12}}} \sum_{n_d,l_d,j_d,m_{j_d},m_{t_d}} \sum_{m_{l_d}} \sum_{m_{s_d}} \sum_{K,M_K} \sum_{N_{cm},L_{cm},N_3,L_3} \sum_{M_{L_{cm}},M_{L_3}} \sum_{J_3,M_{J_3}} \sum_{J_{123},M_{J_{123}}} \sum_{T_{123},M_{T_{123}}} \sum_{i_{123}} \sum_{m'_{l_d}} \sum_{m'_{s_d}} \sum_{K',M'_K} \sum_{N'_3,L'_3} \sum_{M'_{L_3}} \sum_{J'_3,M'_{J_3}} \sum_{i'_{123}} \\
&\quad \mathrm{c}\begin{pmatrix} l_d & \frac{1}{2} & \left| & j_d \\ m_{l_d} & m_{s_d} & \right| & m_{j_d} \end{pmatrix} \mathrm{c}\begin{pmatrix} l_d & \frac{1}{2} & \left| & j_d \\ m'_{l_d} & m'_{s_d} & \right| & m_{j_d} \end{pmatrix} \mathrm{c}\begin{pmatrix} 0 & l_d & \left| & K \\ 0 & m_{l_d} & \right| & M_K \end{pmatrix} \mathrm{c}\begin{pmatrix} 0 & l_d & \left| & K' \\ 0 & m'_{l_d} & \right| & M'_K \end{pmatrix} \mathrm{c}\begin{pmatrix} L_{cm} & L_3 & \left| & K \\ M_{L_{cm}} & M_{L_3} & \right| & M_K \end{pmatrix} \\
&\quad \mathrm{c}\begin{pmatrix} L_{cm} & L'_3 & \left| & K' \\ M_{L_{cm}} & M'_{L_3} & \right| & M'_K \end{pmatrix} \mathrm{c}\begin{pmatrix} L_3 & \frac{1}{2} & \left| & J_3 \\ M_{L_3} & m_{s_d} & \right| & M_{J_3} \end{pmatrix} \mathrm{c}\begin{pmatrix} L'_3 & \frac{1}{2} & \left| & J'_3 \\ M'_{L_3} & m'_{s_d} & \right| & M'_{J_3} \end{pmatrix} \mathrm{c}\begin{pmatrix} J_{12} & J_3 & \left| & J_{123} \\ M_{J_{12}} & M_{J_3} & \right| & M_{J_{123}} \end{pmatrix} \mathrm{c}\begin{pmatrix} J_{12} & J'_3 & \left| & J_{123} \\ M_{J_{12}} & M'_{J_3} & \right| & M_{J_{123}} \end{pmatrix} \\
&\quad \mathrm{c}\begin{pmatrix} T_{12} & \frac{1}{2} & \left| & T_{123} \\ M_{T_{12}} & m_{t_d} & \right| & M_{T_{123}} \end{pmatrix} \mathrm{c}\begin{pmatrix} T_{12} & \frac{1}{2} & \left| & T_{123} \\ M_{T_{12}} & m_{t_d} & \right| & M_{T_{123}} \end{pmatrix} \ll N_{cm}L_{cm}, N_3L_3|00, n_dl_d; K \gg_3 \ll N_{cm}L_{cm}, N'_3L'_3|00, n_dl_d; K' \gg_3 \\
&\quad \tilde{c}^{E_{123},J_{123},T_{123},i_{123}}_{k_{123}} \tilde{c}^{E'_{123},J_{123},T_{123},i'_{123}}_{k'_{123}} {}_a\left\langle E'_{123} i'_{123} J_{123} T_{123}\right| V_{4N} \left|E_{123} i_{123} J_{123} T_{123}\right\rangle_a ,
\end{aligned}
\tag{4.51}
$$

where we used the following properties of the four-body interaction to simplify the expression: It is independent of the four-body center-of-mass part, eliminating three sums. Furthermore, the four-body interaction is independent of the projection quantum numbers and diagonal in J_{123} and T_{123}, which removes four sums.

We can further simplify this expression if we assume a closed-shell nucleus with the same number of protons and neutrons. We start by carrying out the sums over j_d, m_{j_d}, m_{t_d}, $M_{T_{12}}$, $M_{J_{12}}$ and $M_{J_{123}}$ using the orthogonality relations of the CGCs (Eqs. 3.7, 3.8). For the last two sums over $M_{J_{12}}$ and $M_{J_{123}}$ a symmetry transformation of the CGCs is necessary (Eq. 3.10) before carrying them out, which yields a factor of $\hat{J}_{123}^2\hat{J}_3^{-2}$. The resulting δ-functions are used to reduce the number of sums:

$$
\begin{aligned}
&{}_a\left\langle E'_{12}, i'_{12}, J_{12}, T_{12}\right| V_{3N}^{eff} \left|E_{12}, i_{12}, J_{12}, T_{12}\right\rangle_a \\
&= 4\, \hat{J}_{12}^{-2}\hat{T}_{12}^{-2} \sum_{n_d,l_d} \sum_{m_{l_d}} \sum_{m_{s_d}} \sum_{K,M_K} \sum_{N_{cm},L_{cm},N_3,L_3} \sum_{M_{L_{cm}},M_{L_3}} \sum_{J_3,M_{J_3}} \sum_{J_{123}} \sum_{T_{123},M_{T_{123}}} \sum_{i_{123}} \sum_{K',M'_K} \sum_{N'_3,L'_3} \sum_{M'_{L_3}} \sum_{i'_{123}} \hat{J}_{123}^2\hat{J}_3^{-2} \\
&\quad \mathrm{c}\begin{pmatrix} 0 & l_d & \left| & K \\ 0 & m_{l_d} & \right| & M_K \end{pmatrix} \mathrm{c}\begin{pmatrix} 0 & l_d & \left| & K' \\ 0 & m_{l_d} & \right| & M'_K \end{pmatrix} \mathrm{c}\begin{pmatrix} L_{cm} & L_3 & \left| & K \\ M_{L_{cm}} & M_{L_3} & \right| & M_K \end{pmatrix} \\
&\quad \mathrm{c}\begin{pmatrix} L_{cm} & L'_3 & \left| & K' \\ M_{L_{cm}} & M'_{L_3} & \right| & M'_K \end{pmatrix} \mathrm{c}\begin{pmatrix} L_3 & \frac{1}{2} & \left| & J_3 \\ M_{L_3} & m_{s_d} & \right| & M_{J_3} \end{pmatrix} \mathrm{c}\begin{pmatrix} L'_3 & \frac{1}{2} & \left| & J_3 \\ M'_{L_3} & m_{s_d} & \right| & M_{J_3} \end{pmatrix} \\
&\quad \ll N_{cm}L_{cm}, N_3L_3|00, n_dl_d; K \gg_3 \ll N_{cm}L_{cm}, N'_3L'_3|00, n_dl_d; K' \gg_3 \\
&\quad \tilde{c}^{E_{123},J_{123},T_{123},i_{123}}_{k_{123}} \tilde{c}^{E'_{123},J_{123},T_{123},i'_{123}}_{k'_{123}} {}_a\left\langle E'_{123} i'_{123} J_{123} T_{123}\right| V_{4N} \left|E_{123} i_{123} J_{123} T_{123}\right\rangle_a .
\end{aligned}
\tag{4.52}
$$

We continue with the sums over m_{s_d} and M_{J_3}, again using the symmetry relation for the CGCs, yielding a factor of $\hat{L}_3^{-2}\hat{J}_3^2$.

$$
\begin{aligned}
&= 4\, \hat{J}_{12}^{-2}\hat{T}_{12}^{-2} \sum_{n_d,l_d} \sum_{m_{l_d}} \sum_{K,M_K} \sum_{N_{cm},L_{cm},N_3,L_3} \sum_{M_{L_{cm}},M_{L_3}} \sum_{J_3} \sum_{J_{123}} \sum_{T_{123},M_{T_{123}}} \sum_{i_{123}} \sum_{K',M'_K} \sum_{N'_3} \sum_{i'_{123}} \hat{J}_{123}^2\hat{L}_3^{-2} \\
&\quad \mathrm{c}\begin{pmatrix} 0 & l_d & \left| & K \\ 0 & m_{l_d} & \right| & M_K \end{pmatrix} \mathrm{c}\begin{pmatrix} 0 & l_d & \left| & K' \\ 0 & m_{l_d} & \right| & M'_K \end{pmatrix} \mathrm{c}\begin{pmatrix} L_{cm} & L_3 & \left| & K \\ M_{L_{cm}} & M_{L_3} & \right| & M_K \end{pmatrix} \mathrm{c}\begin{pmatrix} L_{cm} & L_3 & \left| & K' \\ M_{L_{cm}} & M_{L_3} & \right| & M'_K \end{pmatrix} \\
&\quad \ll N_{cm}L_{cm}, N_3L_3|00, n_dl_d; K \gg_3 \ll N_{cm}L_{cm}, N'_3L_3|00, n_dl_d; K' \gg_3 \\
&\quad \tilde{c}^{E_{123},J_{123},T_{123},i_{123}}_{k_{123}} \tilde{c}^{E'_{123},J_{123},T_{123},i'_{123}}_{k'_{123}} {}_a\left\langle E'_{123} i'_{123} J_{123} T_{123}\right| V_{4N} \left|E_{123} i_{123} J_{123} T_{123}\right\rangle_a .
\end{aligned}
\tag{4.53}
$$

Furthermore, we carry out the sums over $M_{L_{cm}}$, M_{L_3}, m_{l_d}, and M_K. Again, we use the symmtry relation from Eq. (3.10) to reorder entries in CGCs, yielding a factor $\hat{K}^2$.

$$
\begin{aligned}
&{}_a\left\langle E'_{12}, i'_{12}, J_{12}, T_{12}\right| V_{3N}^{eff} \left|E_{12}, i_{12}, J_{12}, T_{12}\right\rangle_a \\
&\quad = 4\,\hat{J}_{12}^{-2}\hat{T}_{12}^{-2} \sum_{n_d,l_d}\sum_{K}\sum_{N_{cm},L_{cm},N_3,L_3}\sum_{J_3}\sum_{J_{123}}\sum_{T_{123},M_{T_{123}}}\sum_{i_{123}}\sum_{N'_3}\sum_{i'_{123}} \hat{J}_{123}^2 \hat{L}_3^{-2} \hat{K}^2 \\
&\qquad \ll N_{cm}L_{cm}, N_3L_3|00, n_dl_d; K \gg_3 \ll N_{cm}L_{cm}, N'_3L_3|00, n_dl_d; K \gg_3 \\
&\qquad \tilde{c}_{k_{123}}^{E_{123},J_{123},T_{123},i_{123}} \tilde{c}_{k'_{123}}^{E'_{123},J_{123},T_{123},i'_{123}} \,{}_a\left\langle E'_{123} i'_{123} J_{123} T_{123}\right| V_{4N} \left|E_{123} i_{123} J_{123} T_{123}\right\rangle_a .
\end{aligned}
\tag{4.54}
$$

Finally, the sum over $M_{T_{123}}$ is carried out as well, as nothing depends on this projection quantum number anymore. From the energy conservation of the HOBs we can also deduce that $N_3 = N'_3$. From the HOBs we can see that $K = l_d$.

$$
\begin{aligned}
&= 4\,\hat{J}_{12}^{-2}\hat{T}_{12}^{-2} \sum_{n_d,l_d}\sum_{N_{cm},L_{cm},N_3,L_3}\sum_{J_3}\sum_{J_{123}}\sum_{T_{123}}\sum_{i_{123}}\sum_{i'_{123}} \hat{J}_{123}^2 \hat{T}_{123}^2 \hat{L}_3^{-2} \hat{l}_d^2 \\
&\quad \ll N_{cm}L_{cm}, N_3L_3|00, n_dl_d; l_d \gg_3 \ll N_{cm}L_{cm}, N_3L_3|00, n_dl_d; l_d \gg_3 \\
&\quad \tilde{c}_{k_{123}}^{E_{123},J_{123},T_{123},i_{123}} \tilde{c}_{k'_{123}}^{E'_{123},J_{123},T_{123},i'_{123}} \,{}_a\left\langle E'_{123} i'_{123} J_{123} T_{123}\right| V_{4N} \left|E_{123} i_{123} J_{123} T_{123}\right\rangle_a .
\end{aligned}
\tag{4.55}
$$

For closed shell nuclei with the same number of protons and neutron we end up with Eq. (4.55), which is a rather simple formula that does not take much computation time to evaluate. The result is an interaction in a three-body Jacobi basis, which can be handled with the existing three-body framework. It is therefore well suited to gauge the effect of four-body forces quickly without the time consumption necessary for incorporating the four-body forces in a many-body calculation. However, this approach is based on multiple uncontrolled approximations that can greatly influence the results, making the explicit inclusion of four-body forces the preferred solution.

4.6 Representing Few-Body Interactions in a Many-Body Basis

Having discussed an approximate approach for reducing the four-body interaction to a three-body interaction, we will now do the opposite and represent few-body interactions in a higher-body space. Being able to express interactions in an A-body space is mandatory for any many-body calculation. No approximations are needed for representing few-body interactions in a many-body basis. We will first discuss some basic principles, independent of the actual basis, and then continue with the rules for a few- to many-body conversion in the m-scheme. Afterwards we will discuss embedding matrix elements given in two- and three-body Jacobi basis in a three- or four-body Jacobi basis. As we already discussed, constructing a many-body Jacobi basis is not feasible, currently limiting us to a four-body Jacobi basis. In the next sections we use the following notation:

- Upper indices in square brackets indicate irreducible n-body content, e.g., an upper index [3] indicates an operator that can only be represented in spaces with 3 or more particles.
- Lower indices indicate the particle spaces the operator acts in, e.g., $V_{2,4}^{[2]}$ is a irreducible two-body interaction, which acts in particle spaces 2 and 4. Obviously, an operator that acts in particle space 4 requires a Hilbert space with four or more particles.

If we want to embed an irreducible N-body interaction in A-body space, with $N < A$, we simply sum over all possible contributions of the irreducible N-body interaction in the A-body Hilbert space:

$$
V_{1,2,\ldots,A}^{[N]} = \sum_{\substack{k_1,k_2,\ldots,k_N \\ k_1<k_2<\cdots<k_N}} V_{k_1,k_2,\ldots,k_N}^{[N]},
\tag{4.56}
$$

e.g., for $A = 4$ and $N = 2$:

$$
V_{1,2,3,4}^{[2]} = V_{1,2}^{[2]} + V_{1,3}^{[2]} + V_{1,4}^{[2]} + V_{2,3}^{[2]} + V_{2,4}^{[2]} + V_{3,4}^{[2]}.
\tag{4.57}
$$

The formula becomes simpler if we look at matrix elements of antisymmetric states. As all the contributions we sum up are identical in that case, we simply get a factor instead of a sum:

$$
{}_a\left\langle \Psi'\right| V_{1,2,\ldots,A}^{[N]} \left|\Psi\right\rangle_a = \binom{A}{N} \,{}_a\left\langle \Psi'\right| V_{1,2,\ldots,N}^{[N]} \left|\Psi\right\rangle_a ,
\tag{4.58}
$$

where $|\Psi\rangle_a$ and $|\Psi'\rangle_a$ are antisymmetric A-body states. For example, transforming a two-body interaction to a four-body one yields

$$ {}_a\langle\Psi'|\, V^{[2]}_{1,2,3,4}\,|\Psi\rangle_a = 6\ {}_a\langle\Psi'|\, V^{[2]}_{1,2}\,|\Psi\rangle_a\,. \tag{4.59} $$

It is important to note that Eq. (4.58) only holds if one has an irreducible N-body operator that is represented in an N-body space. If we, for instance, embed an irreducible two-body interaction in three-body space and then use this representation in three-body space and embed it in four-body space with Eq. (4.58), assuming the representation of the irreducible two-body interaction in three-body space acts as if it was an irreducible three-body interaction, we obtain

$$ {}_a\langle\Psi'|\, V'^{[2]}_{1,2,3,4}\,|\Psi\rangle_a = 4\cdot 3\ {}_a\langle\Psi'|\, V^{[2]}_{1,2}\,|\Psi\rangle_a \tag{4.60} $$

$$ = 2\ {}_a\langle\Psi'|\, V^{[2]}_{1,2,3,4}\,|\Psi\rangle_a\,, \tag{4.61} $$

which is obviously not the result we anticipated. The same problem arises when representing irreducible one-body operator, e.g., the kinetic energy operator, in an A-body space via representations in two- or three-body space. In a simple case as stated above, we can easily fix the factor. However, if we represent an irreducible two-body interaction in three-body space and combine it with an irreducible three-body interaction, it is not possible to embed the combined interaction in a many-body space. Therefore, we have to handle irreducible one-, two-, three- and four-body interactions separately until we combine them to a total interaction in the A-body space for the many-body calculation.

In the following two sections we will use Eq. (4.58) for representing interactions in A-body space using the m-scheme and representing irreducible two- or three-body interactions in three- or four-body Jacobi basis.

4.6.1 m-Scheme

When applying Eq. (4.58) to the m-scheme, we have to evaluate the matrix element on the right-hand side. We start with a discussion of an irreducible two-body interaction, which is represented in two-body space. We embed it in three-body space, obtaining the following three-body matrix elements:

$$ {}_a\langle a'b'c'|\, V^{[2]}_{1,2,3}\,|abc\rangle_a = 3\ {}_a\langle a'b'c'|\, V^{[2]}_{1,2}\,|abc\rangle_a \tag{4.62} $$

To evaluate the matrix element on the right-hand side of Eq. (4.62), we have to antisymmetrize bra and ket explicitly.

$$ |abc\rangle_a = \frac{1}{\sqrt{3!}}\sum_{\mathcal{P}} \mathrm{sgn}(\mathcal{P})\,|\mathcal{P}_a\mathcal{P}_b\mathcal{P}_c\rangle\,, \tag{4.63} $$

where we sum over all possible permutations $\mathcal{P}$ of a, b, and c. For the two-body matrix elements we need antisymmetric two-body states:

$$ = \frac{1}{\sqrt{3}}\left(\frac{1}{\sqrt{2!}}\sum_{\tilde{\mathcal{P}}}\mathrm{sgn}\left(\tilde{\mathcal{P}}\right)|\tilde{\mathcal{P}}_a\tilde{\mathcal{P}}_b\rangle\,|c\rangle - \frac{1}{\sqrt{2!}}\sum_{\tilde{\mathcal{P}}}\mathrm{sgn}\left(\tilde{\mathcal{P}}\right)|\tilde{\mathcal{P}}_a\tilde{\mathcal{P}}_c\rangle\,|b\rangle + \frac{1}{\sqrt{2!}}\sum_{\tilde{\mathcal{P}}}\mathrm{sgn}\left(\tilde{\mathcal{P}}\right)|\tilde{\mathcal{P}}_b\tilde{\mathcal{P}}_c\rangle\,|a\rangle\right) \tag{4.64} $$

$$ = \frac{1}{\sqrt{3}}\left(|ab\rangle_a\,|c\rangle - |ac\rangle_a\,|b\rangle + |bc\rangle_a\,|a\rangle\right), \tag{4.65} $$

where the permutations only act on the first two particles. Inserting this expansion in Eq. (4.62) yields

$$ {}_a\langle a'b'c'|\, V^{[2]}_{1,2,3}\,|abc\rangle_a = 3\frac{1}{\sqrt{3}}\left({}_a\langle a'b'|\,\langle c'| - {}_a\langle a'c'|\,\langle b'| + {}_a\langle b'c'|\,\langle a'|\right) V^{[2]}_{1,2}\,\frac{1}{\sqrt{3}}\left(|ab\rangle_a\,|c\rangle - |ac\rangle_a\,|b\rangle + |bc\rangle_a\,|a\rangle\right) \tag{4.66} $$

$$ \begin{aligned} = {}& {}_a\langle a'b'|V^{[2]}_{1,2}|ab\rangle_a\,\delta_{c,c'} - {}_a\langle a'b'|V^{[2]}_{1,2}\,|ac\rangle_a\,\delta_{b,c'} + {}_a\langle a'b'|V^{[2]}_{1,2}\,|bc\rangle_a\,\delta_{a,c'} \\ & - {}_a\langle a'c'|V^{[2]}_{1,2}\,|ab\rangle_a\,\delta_{c,b'} + {}_a\langle a'c'|V^{[2]}_{1,2}|ac\rangle_a\,\delta_{b,b'} - {}_a\langle a'c'|V^{[2]}_{1,2}\,|bc\rangle_a\,\delta_{a,b'} \\ & + {}_a\langle b'c'|V^{[2]}_{1,2}\,|ab\rangle_a\,\delta_{c,a'} - {}_a\langle b'c'|V^{[2]}_{1,2}\,|ac\rangle_a\,\delta_{b,a'} + {}_a\langle b'c'|V^{[2]}_{1,2}|bc\rangle_a\,\delta_{a,a'}\,. \end{aligned} \tag{4.67} $$

For evaluating the expression, the states in bra and ket are usually reordered. All single-particle states that can be found in both bra and ket are reordered to the right side so that they have the same position in bra and ket, e.g.,

$$ {}_a\langle bca'|\, V^{[2]}_{1,2,3}\,|bac\rangle_a \to -\,{}_a\langle a'bc|\, V^{[2]}_{1,2,3}\,|abc\rangle_a\,, \tag{4.68} $$

where the states b and c are identical in bra and ket, while the states a and a' differ. Afterwards we can use Eq. (4.67), where only the parts marked red can be non-zero. Using these ordered matrix elements, we can easily find sums for representing irreducible two-, three-, or four-body interactions in an A-body basis.

Two additional examples are presented below, where we derived the matrix elements of irreducible two- and three-body interactions in the four-body m-scheme. Both of them only work for matrix elements that are ordered as discussed.

$$\begin{aligned}{}_a\langle a'b'c'd'|\, V^{[2]}_{1,2,3,4}\,|abcd\rangle_a = {}& {}_a\langle a'b'|V^{[2]}_{1,2}|ab\rangle_a\,\delta_{c,c'}\delta_{d,d'} + {}_a\langle a'c'|V^{[2]}_{1,2}|ac\rangle_a\,\delta_{b,b'}\delta_{d,d'} + {}_a\langle a'd'|V^{[2]}_{1,2}|ad\rangle_a\,\delta_{b,b'}\delta_{c,c'} \\ & + {}_a\langle b'c'|V^{[2]}_{1,2}|bc\rangle_a\,\delta_{a,a'}\delta_{d,d'} + {}_a\langle b'd'|V^{[2]}_{1,2}|bd\rangle_a\,\delta_{a,a'}\delta_{c,c'} + {}_a\langle c'd'|V^{[2]}_{1,2}|cd\rangle_a\,\delta_{a,a'}\delta_{b,b'}. \end{aligned} \tag{4.69}$$

$$\begin{aligned}{}_a\langle a'b'c'd'|\, V^{[3]}_{1,2,3,4}\,|abcd\rangle_a = {}& {}_a\langle a'b'c'|V^{[3]}_{1,2,3}|abc\rangle_a\,\delta_{d,d'} + {}_a\langle a'b'd'|V^{[3]}_{1,2,3}|abd\rangle_a\,\delta_{c,c'} + {}_a\langle a'c'd'|V^{[3]}_{1,2,3}|acd\rangle_a\,\delta_{b,b'} \\ & + {}_a\langle b'c'd'|V^{[3]}_{1,2,3}|bcd\rangle_a\,\delta_{a,a'} \end{aligned} \tag{4.70}$$

These formulae can be constructed easily, as we simply sum over all possible combinations for the two- or three-body interaction using the states of our A-body matrix element. A calculation for an A-body basis using this method is straightforward.

4.6.2 Jacobi Basis

In this section we derive the transformation of an operator represented in the three-body Jacobi basis to a representation in four-body Jacobi basis. Furthermore, we present formulae for representing an interaction in three- and four-body Jacobi basis, if the interaction is expressed in the two-body Jacobi basis. First of all, we need to transform the antisymmetric four-body Jacobi basis by making the antisymmetry explicit and separating the quantum numbers involving the first three particles from the quantum numbers involving the fourth particle. We omit the center-of-mass part, as we do not change it.

$$\begin{aligned}&\left|E_{123}i_{123}J_{123}M_{J_{123}}T_{123}M_{T_{123}}\right\rangle \\ &= \sum_{k_{123}} \tilde{c}^{E_{123},J_{123},T_{123},i_{123}}_{k_{123}} \left|E_{123}J_{123}M_{J_{123}}T_{123}M_{T_{123}}k_{123}\right\rangle \qquad (4.71) \\ &= \sum_{k_{123}} \tilde{c}^{E_{123},J_{123},T_{123},i_{123}}_{k_{123}} \left|E_{12}i_{12}N_3;\left[J_{12}\left(L_3\tfrac{1}{2}\right)J_3\right]J_{123}M_{J_{123}};\left(T_{12}\tfrac{1}{2}\right)T_{123}M_{T_{123}}\right\rangle, \qquad (4.72)\end{aligned}$$

We decouple the total relative angular momentum and the total isospin using CGCs:

$$\begin{aligned}&= \sum_{k_{123}} \sum_{M_{J_{12}},M_{J_3}} \sum_{M_{T_{12}},m_{t_3}} \tilde{c}^{E_{123},J_{123},T_{123},i_{123}}_{k_{123}} \mathrm{c}\begin{pmatrix} J_{12} & J_3 & J_{123} \\ M_{J_{12}} & M_{J_3} & M_{J_{123}}\end{pmatrix} \mathrm{c}\begin{pmatrix} T_{12} & \frac{1}{2} & T_{123} \\ M_{T_{12}} & m_{t_3} & M_{T_{123}}\end{pmatrix} \\ &\quad \left|E_{12}i_{12}J_{12}M_{J_{12}}T_{12}M_{T_{12}}\right\rangle_a \left|N_3;\left(L_3\tfrac{1}{2}\right)J_3M_{J_3};\tfrac{1}{2}m_{t_3}\right\rangle \end{aligned} \tag{4.73}$$

For deriving the matrix elements, we use Eq. (4.58):

$$\begin{aligned}&{}_a\left\langle E'_{123}i'_{123}J'_{123}M'_{J_{123}}T'_{123}M'_{T_{123}}\right| V^{[3]}_{1,2,3,4}\left|E_{123}i_{123}J_{123}M_{J_{123}}T_{123}M_{T_{123}}\right\rangle_a \\ &= 4\ {}_a\left\langle E'_{123}i'_{123}J'_{123}M'_{J_{123}}T'_{123}M'_{T_{123}}\right| V^{[3]}_{1,2,3}\left|E_{123}i_{123}J_{123}M_{J_{123}}T_{123}M_{T_{123}}\right\rangle_a, \end{aligned} \tag{4.74}$$

where we omitted the center-of-mass part as it is irrelevant. We change the basis by inserting Eq. (4.73).

$$\begin{aligned}&= 4 \sum_{k_{123}} \sum_{M_{J_{12}},M_{J_3}} \sum_{M_{T_{12}},m_{t_3}} \sum_{k'_{123}} \sum_{M'_{J_{12}},M'_{J_3}} \sum_{M'_{T_{12}},m'_{t_3}} \tilde{c}^{E_{123},J_{123},T_{123},i_{123}}_{k_{123}} \tilde{c}^{E'_{123},J'_{123},T'_{123},i'_{123}}_{k'_{123}} \\ &\quad \mathrm{c}\begin{pmatrix} J_{12} & J_3 & J_{123} \\ M_{J_{12}} & M_{J_3} & M_{J_{123}}\end{pmatrix} \mathrm{c}\begin{pmatrix} T_{12} & \frac{1}{2} & T_{123} \\ M_{T_{12}} & m_{t_3} & M_{T_{123}}\end{pmatrix} \mathrm{c}\begin{pmatrix} J'_{12} & J'_3 & J'_{123} \\ M'_{J_{12}} & M'_{J_3} & M'_{J_{123}}\end{pmatrix} \mathrm{c}\begin{pmatrix} T'_{12} & \frac{1}{2} & T'_{123} \\ M'_{T_{12}} & m'_{t_3} & M'_{T_{123}}\end{pmatrix} \\ &\quad {}_a\left\langle E'_{12}i'_{12}J'_{12}M'_{J_{12}}T'_{12}M'_{T_{12}}\right| \left\langle N'_3;\left(L'_3\tfrac{1}{2}\right)J'_3M'_{J_3};\tfrac{1}{2}m'_{t_3}\right| V^{[3]}_{1,2,3}\left|E_{12}i_{12}J_{12}M_{J_{12}}T_{12}M_{T_{12}}\right\rangle_a \left|N_3;\left(L_3\tfrac{1}{2}\right)J_3M_{J_3};\tfrac{1}{2}m_{t_3}\right\rangle. \end{aligned} \tag{4.75}$$

As the irreducible three-body interaction does not act on the quantum numbers involving the fourth particle, i.e., corresponding to the third Jacobi coordinate, we obtain δ-functions for this quantum numbers. Furthermore we use the following properties ouf our interaction to simplify the expression: The interaction is diagonal in angular momentum J_{12} and isospin T_{12} and independent of projection quantum numbers.

$$
\begin{aligned}
&= 4 \sum_{k_{123}} \sum_{M_{J_{12}}, M_{J_3}} \sum_{M_{T_{12}}, m_{t_3}} \sum_{k'_{123}} \sum_{M'_{J_{12}}, M'_{J_3}} \sum_{M'_{T_{12}}, m'_{t_3}} \delta_{J'_{12}, J_{12}} \delta_{T'_{12}, T_{12}} \delta_{N'_3, N_3} \delta_{L'_3, L_3} \delta_{J'_3, J_3} \delta_{M'_{J_3}, M_{J_3}} \delta_{m'_{t_3}, m_{t_3}} \delta_{M'_{J_{12}}, M_{J_{12}}} \delta_{M'_{T_{12}}, M_{T_{12}}} \\
&\quad \tilde{c}^{E_{123}, J_{123}, T_{123}, i_{123}}_{k_{123}} \tilde{c}^{E'_{123}, J'_{123}, T'_{123}, i'_{123}}_{k'_{123}} \\
&\quad \mathrm{c}\begin{pmatrix} J_{12} & J_3 & J_{123} \\ M_{J_{12}} & M_{J_3} & M_{J_{123}} \end{pmatrix} \mathrm{c}\begin{pmatrix} T_{12} & \frac{1}{2} & T_{123} \\ M_{T_{12}} & m_{t_3} & M_{T_{123}} \end{pmatrix} \mathrm{c}\begin{pmatrix} J'_{12} & J'_3 & J'_{123} \\ M'_{J_{12}} & M'_{J_3} & M'_{J_{123}} \end{pmatrix} \mathrm{c}\begin{pmatrix} T'_{12} & \frac{1}{2} & T'_{123} \\ M'_{T_{12}} & m'_{t_3} & M'_{T_{123}} \end{pmatrix} \\
&\quad {}_a\left\langle E'_{12} i'_{12} J_{12} T_{12} \middle| V^{[3]}_{1,2,3} \middle| E_{12} i_{12} J_{12} T_{12} \right\rangle_a .
\end{aligned} \tag{4.76}
$$

We can use the δ-functions to remove some sums. Furthermore, the orthogonality relation of the CGCs can be used to sum over the projection quantum numbers, yielding:

$$
\begin{aligned}
&= 4 \sum_{k_{123}} \sum_{k'_{123}} \delta_{J_{12}, J'_{12}} \delta_{T_{12}, T'_{12}} \delta_{N_3, N'_3} \delta_{L_3, L'_3} \delta_{J_3, J'_3} \delta_{N_{cm}, N'_{cm}} \delta_{L_{cm}, L'_{cm}} \delta_{M_{L_{cm}}, M'_{L_{cm}}} \delta_{T_{123}, T'_{123}} \delta_{M_{T_{123}}, M'_{T_{123}}} \delta_{J_{123}, J'_{123}} \delta_{M_{J_{123}}, M'_{J_{123}}} \\
&\quad \tilde{c}^{E_{123}, J_{123}, T_{123}, i_{123}}_{k_{123}} \tilde{c}^{E'_{123}, J_{123}, T_{123}, i'_{123}}_{k'_{123}} {}_a\left\langle E'_{12} J_{12} T_{12} i'_{12} \middle| V_{1,2,3} \middle| E_{12} J_{12} T_{12} i_{12} \right\rangle_a .
\end{aligned} \tag{4.77}
$$

The δ-functions $\delta_{T_{123}, T'_{123}}$, $\delta_{M_{T_{123}}, M'_{T_{123}}}$, $\delta_{J_{123}, J'_{123}}$ and $\delta_{M_{J_{123}}, M'_{J_{123}}}$ reflect all the properties of the interaction in four-body space. We get an interaction that is independent of projection quantum numbers, as they do not have any influence on the CFPs or the three-body matrix element. Furthermore, the interaction is diagonal in four-body isospin and angular momentum. Using these properties, we can formulate a shortened version of the formula above:

$$
\begin{aligned}
&{}_a\left\langle E'_{123} J_{123} T_{123} i'_{123} \middle| V^{[3]}_{1,2,3,4} \middle| E_{123} J_{123} T_{123} i_{123} \right\rangle_a \\
&\quad = 4 \sum_{k_{123}} \sum_{k'_{123}} \delta_{J_{12}, J'_{12}} \delta_{T_{12}, T'_{12}} \delta_{N_3, N'_3} \delta_{L_3, L'_3} \delta_{J_3, J'_3} \tilde{c}^{E_{123}, J_{123}, T_{123}, i_{123}}_{k_{123}} \tilde{c}^{E'_{123}, J_{123}, T_{123}, i'_{123}}_{k'_{123}} {}_a\left\langle E'_{12} J_{12} T_{12} i'_{12} \middle| V^{[3]}_{1,2,3} \middle| E_{12} J_{12} T_{12} i_{12} \right\rangle_a
\end{aligned} \tag{4.78}
$$

In a similar fashion irreducible two-body matrix elements can be represented in three- and four-body space. We assume three- and higher-body matrix elements in Jacobi basis to be independent of the isospin projection quantum number. When representing a two-body interaction in a higher-body Jacobi basis, we need to approximate the two-body interaction to be independent of the isospin projection number as well. However, this approximation is just used when transforming the interaction in Jacobi basis, it is unnecessary in the m-scheme.

$$
\begin{aligned}
&{}_a\left\langle E'_{12} J_{12} T_{12} i'_{12} \middle| V^{[2]}_{1,2,3} \middle| E_{12} J_{12} T_{12} i_{12} \right\rangle_a \\
&\quad = 6 \sum_{k_{12}} \sum_{k'_{12}} \delta_{J_1, J'_1} \delta_{T_1, T'_1} \delta_{N_2, N'_2} \delta_{L_2, L'_2} \delta_{J_2, J'_2} c^{E_{12}, J_{12}, T_{12}, i_{12}}_{k_{12}} c^{E'_{12}, J_{12}, T_{12}, i'_{12}}_{k'_{12}} {}_a\left\langle N'_1; \left(L'_1 S'_1\right) J_1; T_1 \middle| V^{[2]}_{1,2} \middle| N_1; \left(L_1 S_1\right) J_1; T_1 \right\rangle_a
\end{aligned} \tag{4.79}
$$

$$
\begin{aligned}
&{}_a\left\langle E'_{123} J_{123} T_{123} i'_{123} \middle| V^{[2]}_{1,2,3,4} \middle| E_{123} J_{123} T_{123} i_{123} \right\rangle_a \\
&\quad = 12 \sum_{k_{123}} \sum_{k'_{123}} \sum_{k_{12}} \sum_{k'_{12}} \delta_{J_{12}, J'_{12}} \delta_{T_{12}, T'_{12}} \delta_{J_1, J'_1} \delta_{T_1, T'_1} \delta_{N_3, N'_3} \delta_{L_3, L'_3} \delta_{J_3, J'_3} \delta_{N_2, N'_2} \delta_{L_2, L'_2} \delta_{J_2, J'_2} \\
&\quad \tilde{c}^{E_{123}, J_{123}, T_{123}, i_{123}}_{k_{123}} \tilde{c}^{E'_{123}, J_{123}, T_{123}, i'_{123}}_{k'_{123}} c^{E_{12}, J_{12}, T_{12}, i_{12}}_{k_{12}} c^{E'_{12}, J_{12}, T_{12}, i'_{12}}_{k'_{12}} {}_a\left\langle N'_1; \left(L'_1 S'_1\right) J_1; T_1 \middle| V_{1,2} \middle| N_1; \left(L_1 S_1\right) J_1; T_1 \right\rangle_a
\end{aligned} \tag{4.80}
$$

Note that the CFPs are needed for the formulae derived above. The calculation of the CFPs takes a lot of effort, which increases with the number of particles, stopping us from representing interactions in a many-body Jacobi basis. Furthermore, the transformations of the matrix elements involve sums over k_{12} or k_{123}. The formulae for representing interactions in the A-body m-scheme (see Sec. 4.6.1) do not need any CFPs or large sums. Therefore, the transformations in m-scheme are much faster than in Jacobi basis and allow an easy construction of matrix elements in an A-body basis.

5 Similarity Renormalization Group

If we use any of our HO bases, e.g., the Jacobi basis, for representing the interaction, the matrix elements of most modern potentials have strong off-diagonal elements, which connect low-lying and high-lying basis states, i.e., states with a low and a high HO energies. The reason can be found in the properties of the interactions themselves, as they all induce strong correlations in the resulting nuclear states. For example, they all feature a strong short-range repulsion which yields short-range correlations. The states in our bases do not contain any correlation and representing correlations with our bases requires high-lying basis states. Furthermore, the coupling between low- and high-lying states is strong and the latter must be included in any many-body calculation. However, incorporating all necessary states poses a problem, as any model space with all these states would be far too large to handle. This can also be seen in the slow-convergence of exact many-body calculations, e.g., NCSM calculations. They converge towards the exact result by increasing the size of the model space and with an interaction in place that induces strong correlations, this convergence is too slow.

There are two possible options to solve the problem described above: We can either use a basis that incorporates correlations, or we can transform the interaction itself. Two typical methods for transforming the interactions are the UCOM and the SRG, both greatly improve the convergence of subsequent many-body calculations [10]. We will focus on the latter, and use it to 'soften' the potential, e.g., reduce the short-range repulsion. In doing so we decouple low-lying and high-lying states and, therefore, improve convergence. Furthermore, we want phase-shifts and observables to be preserved in the low-energy regime when applying the transformation.

5.1 Basic Formulation

For defining and calculating the transformation the following flow equation with the flow parameter α is used:

$$\frac{\mathrm{d}H_\alpha}{\mathrm{d}\alpha} = \left[\eta_\alpha, H_\alpha\right], \tag{5.1}$$

where η_α is an anti-hermitian generator that can be chosen freely. The initial Hamiltonian corresponds to $H_{\alpha=0}$ and a transformed Hamiltonian is obtained by integrating the equation given above. Such a continuous transformation can be performed for any value of α, which offers a simple tool to analyze results obtained with the transformed Hamiltonian:The SRG transformation should not change the results obtained by a subsequent many-body method. Therefore, any result that is obtained with a many-body calculation, which is converged with respect to the model space, should be independent of α. If that is not the case, the observables are changed during the evolution of the flow-equation. To get consistent observables in the first place, any other operator must be evolved as well, yielding a similar flow-equation

$$\frac{\mathrm{d}O_\alpha}{\mathrm{d}\alpha} = \left[\eta_\alpha, O_\alpha\right]. \tag{5.2}$$

However, the generator usually depends on the Hamiltonian, which forces us to evolve the Hamiltonian and any additional operator simultaneously. As the resulting transformation is unitary, it can also be written as

$$H_\alpha = U_\alpha^\dagger H_0 U_\alpha. \tag{5.3}$$

Using the following equation,

$$\frac{\mathrm{d}U_\alpha^\dagger U_\alpha}{\mathrm{d}\alpha} = \frac{\mathrm{d}U_\alpha^\dagger}{\mathrm{d}\alpha} U_\alpha + U_\alpha^\dagger \frac{\mathrm{d}U_\alpha}{\mathrm{d}\alpha} = 0 \tag{5.4}$$

$$\Rightarrow \frac{\mathrm{d}U_\alpha^\dagger}{\mathrm{d}\alpha} = - U_\alpha^\dagger \frac{\mathrm{d}U_\alpha}{\mathrm{d}\alpha} U_\alpha^\dagger, \tag{5.5}$$

we can derive a relation between the unitary operator and the generator.

$$\frac{\mathrm{d}U_\alpha^\dagger H_0 U_\alpha}{\mathrm{d}\alpha} = \frac{\mathrm{d}U_\alpha^\dagger}{\mathrm{d}\alpha} H_0 U_\alpha + U_\alpha^\dagger H_0 \frac{\mathrm{d}U_\alpha}{\mathrm{d}\alpha} \tag{5.6}$$

$$= - U_\alpha^\dagger \frac{\mathrm{d}U_\alpha}{\mathrm{d}\alpha} U_\alpha^\dagger H_0 U_\alpha + U_\alpha^\dagger H_0 U_\alpha U_\alpha^\dagger \frac{\mathrm{d}U_\alpha}{\mathrm{d}\alpha} \tag{5.7}$$

$$= \left[- U_\alpha^\dagger \frac{\mathrm{d}U_\alpha}{\mathrm{d}\alpha}, U_\alpha^\dagger H_0 U_\alpha \right] \tag{5.8}$$

$$\Rightarrow \eta_\alpha = -U_\alpha^\dagger \frac{\mathrm{d}U_\alpha}{\mathrm{d}\alpha}. \tag{5.9}$$

This equation allows to calculate a representation of the unitary transformation operator, which would make it simple to transform any other operator. However, as we only transform the Hamiltonian, using the flow-equation directly is easier.

For any actual calculation the flow equation has to be integrated in a finite model space. Representing the flow equation in a finite model space yields the same equations with one major difference: We have to deal with matrices instead of operators. Choosing a model space imposes two truncations. The SRG induces many-body forces, which will be discussed in detail in the next section. Choosing a basis limits the number of particles and therefore the induced forces we can take into account. In principal, we would have to use an A-body basis for performing a many-body calculation for an A-body nucleus. That is not feasible and we are limited to a four-body basis at present. Secondly, we have to truncate any basis, omitting high-energetic states. This can significantly modify the outcome and the results obtained with such a transformed Hamiltonian should be checked by varying the truncation. The effect of the transformation also strongly depends on the generator. This offers great flexibility and allows to adapt the generator to a specific problem. The original choice by Wegner [30, 31] is a particular simple and intuitive one regarding the diagonalization of the Hamiltonian:

$$\eta_\alpha = \left[\mathrm{diag}\left(H_\alpha\right), H_\alpha\right], \tag{5.10}$$

where $\mathrm{diag}\left(H_\alpha\right)$ is the diagonal part of the Hamiltonian with all off-diagonal matrix elements set to zero in the chosen basis. The obvious fixpoint for the differential equation is a purely diagonal Hamiltonian, as the generator vanishes in that case and, indeed, all off-diagonal matrix elements are suppressed during the evolution making the fixpoint an atractive one [31]. We will, however, use the following generator to achieve a pre-diagonalization in the Jacobi basis:

$$\eta_\alpha = m^2 \left[T_{\mathrm{int}}, H_\alpha\right] \tag{5.11}$$

$$\Rightarrow \frac{\mathrm{d}H_\alpha}{\mathrm{d}\alpha} = m^2 \left(T_{\mathrm{int}} H_\alpha H_\alpha - 2\, H_\alpha T_{\mathrm{int}} H_\alpha + H_\alpha H_\alpha T_{\mathrm{int}}\right), \tag{5.12}$$

where T_{int} is the intrinsic kinetic energy and m is the mass of a nucleon assuming the same mass for protons and neutrons. The factor m^2 fixes the dimension of α to be fm^4. Note that such a choice suppresses the off-diagonal terms as well. Furthermore, such a choice yields results that do not depend on the basis if neglecting the influence of different truncations. This generator is one of the standard choices [10, 32] and although multiple-generators have been put forward, we have so far not discovered one that yields a better convergence of subsequent many-body methods without inducing stronger many-body forces, e.g., see the comparison done by Reinhardt [33]. By choosing a different generator, a transformation can be created that is tailored to a specific problem. Instead of aiming at a pre-diagonalization one can for instance use a generator that evolves the Hamiltonian towards a block-diagonal form as done by Anderson et al. [34].

5.2 Induced Many-Body Forces

One of the main problems encountered using the SRG are induced many-body forces. Even though the original Hamiltonian only had two- and three-body contributions, an evolved Hamiltonian can have up to A-body contributions, if one wants to calculate observables involving A nucleons. In principle, all these parts would have to be calculated during the SRG evolution and then used in the many-body calculation. This is not feasible in general and at the moment we can take into account up to four-body interactions. The truncation is automatically done by choosing a basis. For example, if we evolve a two-body interaction in a three-body basis we will have irreducible two- and three-body parts but induced four-body and higher parts are neglected. The interactions only induce higher-body parts during the SRG evolution, e.g., a two-body interaction does not induce one-body contributions. This means that for the evolution of the irreducible four-body part, the one-, two- and three-body part is necessary, but the three-body part, for instance, is independent of whether or not we include the induced four-body contributions.

In this section we will use the following notation for operators:

- Upper indices in square brackets indicate the irreducible n-body content.
- SRG-evolved operators will be indicated by a tilde and an additional lower index α

- To distinguish between initial two- and three-body interactions the lower indices 'NN' and '3N' are used.

For example, the unevolved interactions are indicated by $V_{\mathrm{NN}}^{[2]}$ and $V_{\mathrm{3N}}^{[3]}$ for the two- and three-body interactions, respectively. Clearly the two-body interaction has irreducible two-body parts only, whereas the three-body interaction has irreducible three-body parts. Note that square brackets do not indicate the basis we are using and $V_{\mathrm{NN}}^{[2]}$ can easily be represented in a four-body basis (see Sec. 4.6.2). After an SRG evolution in two-body space the interaction is denoted by $\tilde{V}_{\mathrm{NN},\alpha}^{[2]}$. If evolving the two-body interaction in three-body space, we also get irreducible three-body interactions denoted by $\tilde{V}_{\mathrm{NN},\alpha}^{[3]}$.

Apart from the interaction we have to take care of the intrinsic kinetic energy in our initial Hamiltonian,

$$H = H^{[2]} + H^{[3]} = T_{\mathrm{int}} + V_{\mathrm{NN}}^{[2]} + V_{\mathrm{3N}}^{[3]}. \tag{5.13}$$

The intrinsic kinetic energy is given by

$$T_{\mathrm{int}} = T - T_{\mathrm{cm}}, \tag{5.14}$$

where T is the total kinetic energy and T_{cm} is the center-of-mass part. It can also be written as

$$T_{\mathrm{int}} = \frac{1}{A\,m} \sum_{i<j} q_{ij}^2, \tag{5.15}$$

where A is the number of nucleons and m is the mass of a nucleon, which we assume to be identical for protons and neutrons. Furthermore, $q_{ij} = \frac{1}{\sqrt{2}} \left(p_i - p_j \right)$ is the relative momentum of two nucleons. Equation (5.15) suggests that the intrinsic kinetic energy is a two-body operator. While that is true for a fixed A, the intrinsic kinetic energy cannot be represented in higher-body bases like other operators, as the factor A needs to be taken into account. We, therefore, omit the upper index for the intrinsic kinetic energy operator. When evolving the Hamiltonian irreducible many-body parts are induced by the intrinsic kinetic energy as well.

$$T_{\mathrm{int}} \xrightarrow{SRG} T_{\mathrm{int}} + \tilde{T}_{\mathrm{int},\alpha}^{[2]} + \tilde{T}_{\mathrm{int},\alpha}^{[3]} + \tilde{T}_{\mathrm{int},\alpha}^{[4]} + \ldots \tag{5.16}$$

For an SRG transformation in four-body space we would write

$$T_{\mathrm{int}} + V_{\mathrm{NN}}^{[2]} + V_{\mathrm{3N}}^{[3]} \xrightarrow{SRG\,(4B)} T_{\mathrm{int}} + \tilde{T}_{\mathrm{int},\alpha}^{[2]} + \tilde{T}_{\mathrm{int},\alpha}^{[3]} + \tilde{T}_{\mathrm{int},\alpha}^{[4]} + \tilde{V}_{\mathrm{NN},\alpha}^{[2]} + \tilde{V}_{\mathrm{NN},\alpha}^{[3]} + \tilde{V}_{\mathrm{NN},\alpha}^{[4]} + \tilde{V}_{\mathrm{3N},\alpha}^{[3]} + \tilde{V}_{\mathrm{3N},\alpha}^{[4]}. \tag{5.17}$$

When transforming interactions we want to have the irreducible two-, three- and four-body parts separate afterwards. There are two main reasons for that. Most importantly, they have to be handled differently during a many-body calculation, as it is impossible to represent a combination of contributions with different irreducible n-body content, e.g., a combination of irreducible two- and three-body contributions, in a higher-body space, as shown in Sec. 4.6. Furthermore, the number of matrix elements increases much faster with the energy for a four-body basis than for a two-body one. By separating the different parts, we can use a higher energy limit for the irreducible two-body part than for any many-body part. We perform a cluster expansion of the evolved Hamiltonian, to achieve a separation of the irreducible two-, three- and four-body parts. The details of such an expansion are discussed in detail in the following sections.

5.2.1 Two-Body Part

We have two different ways for transforming the two-body interaction in the two-body space. The matrix elements that are transformed to the m-scheme and used in a subsequent many-body calculation are transformed in momentum space, see pp. 16 - 19 of Ref. [33].

For using the two-body part in any subtraction scheme we have a different set of matrix elements. As we neglect the dependence on isospin projection for three- and four-body matrix elements, we need to construct an approximate two-body interaction that is independent of the isospin projection quantum numbers as well. The interaction is already constructed to be diagonal in isospin and its projection. We have two possible isospin channels: $T = 0$ and $T = 1$. For the former only one projection quantum number, $M_T = 0$, is possible. The latter has three possible projection quantum numbers and we simply calculate the average of these three matrix elements to obtain one matrix element that is independent of the projection quantum number.

These matrix elements are then evolved in Jacobi basis

$$\left|N_{\mathrm{cm}} L_{\mathrm{cm}} M_{L_{\mathrm{cm}}}; N_1; (L_1 S_1)\, J_1 M_{J_1}; T_1 M_{T_1}\right\rangle,$$

which has been discussed in detail in Sec. 4.1.2, using the following truncation:

$$2\,N_1 + L_1 \leq E_{\mathrm{max}}^{\mathrm{SRG},2}. \tag{5.18}$$

Imposing such a truncation can influence the results that are obtained with a subsequent many-body method and, therefore, it is necessary to check if the results are converged with respect to the SRG model space size, i.e., slightly varying the truncation should not influence the results. The transformation in two-body space only yields irreducible two-body parts:

$$T_{\mathrm{int}} + V_{\mathrm{NN}}^{[2]} \xrightarrow{SRG\,(2B)} T_{\mathrm{int}} + \tilde{T}_{\mathrm{int},\alpha}^{[2]} + \tilde{V}_{\mathrm{NN},\alpha}^{[2]}. \tag{5.19}$$

The initial intrinsic kinetic energy is subtracted after the transformation, as we only need the evolved irreducible two-body part of the interaction for subsequent subtraction schemes that produce higher-body contributions. After transforming them, the matrix elements can be embedded in a three- or four-body basis (see Sec. 4.6.2) and can be used for subtraction schemes afterwards. As the Hamiltonian is diagonal in isospin T_1, angular momentum J_1, and parity π_1, the transformation can be done for each channel separately, where each channel is denoted by the quantum numbers T_1, J_1, and π_1.

5.2.2 Three-Body Part

Three-body matrix elements are exclusively transformed using the Jacobi basis

$$\left|E_{12} i_{12} J_{12} T_{12}\right\rangle_a, \tag{5.20}$$

which has been discussed in detail in Sec. 4.1.3, with the following truncation:

$$E_{12} \leq E_{\mathrm{max}}^{\mathrm{SRG},3}. \tag{5.21}$$

For separating the irreducible three-body parts, we have to subtract the irreducible two-body parts. Doing both transformations,

$$T_{\mathrm{int}} + V_{\mathrm{NN}}^{[2]} \xrightarrow{SRG\,(2B)} T_{\mathrm{int}} + \tilde{T}_{\mathrm{int},\alpha}^{[2]} + \tilde{V}_{\mathrm{NN},\alpha}^{[2]} \tag{5.22}$$

$$T_{\mathrm{int}} + V_{\mathrm{NN}}^{[2]} + V_{\mathrm{3N}}^{[3]} \xrightarrow{SRC\,(3B)} T_{\mathrm{int}} + \tilde{T}_{\mathrm{int},\alpha}^{[2]} + \tilde{T}_{\mathrm{int},\alpha}^{[3]} + \tilde{V}_{\mathrm{NN},\alpha}^{[2]} + \tilde{V}_{\mathrm{NN},\alpha}^{[3]} + \tilde{V}_{\mathrm{3N},\alpha}^{[3]}, \tag{5.23}$$

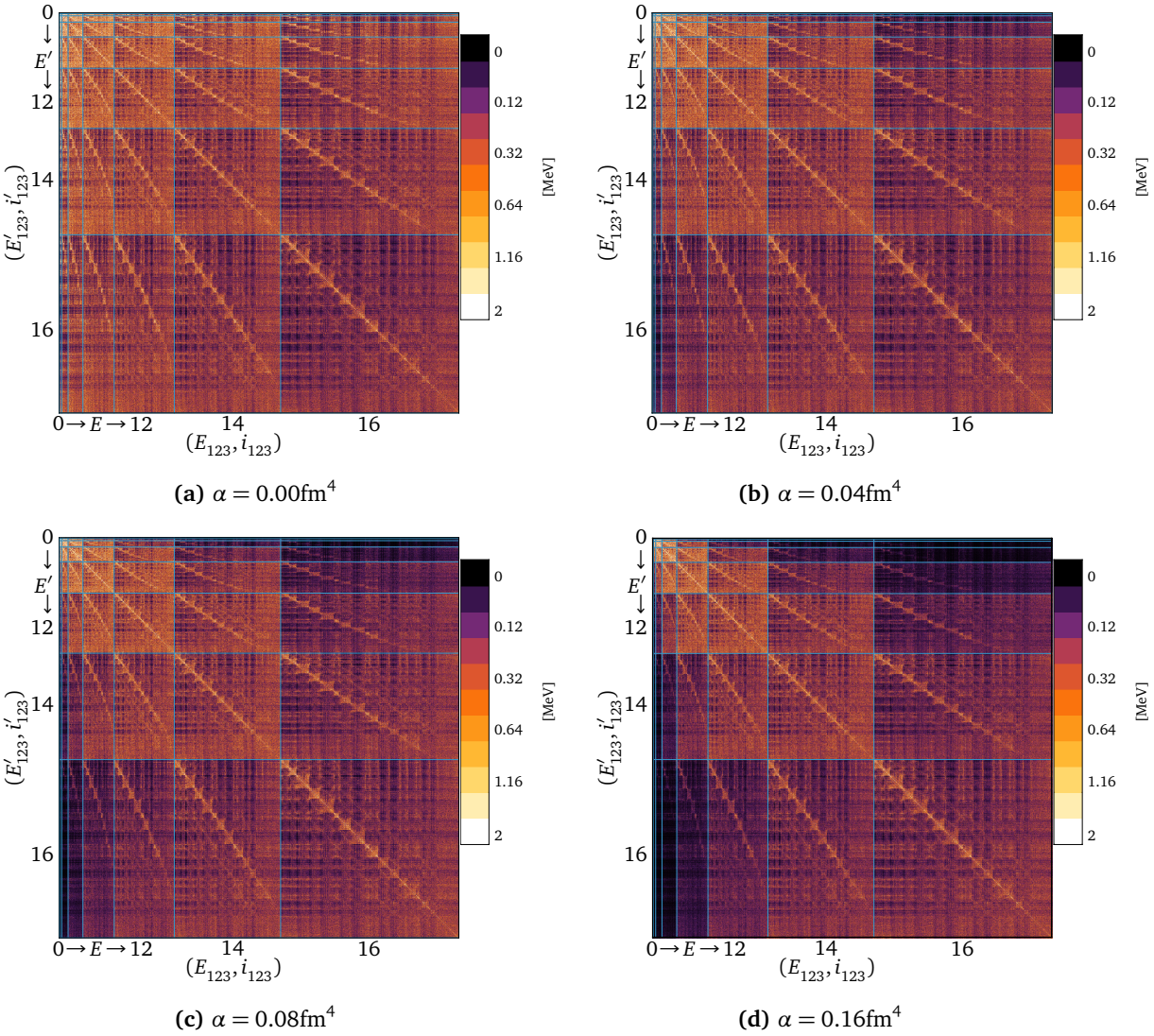
one can easily acquire the desired part $\tilde{T}_{\mathrm{int},\alpha}^{[3]} + \tilde{V}_{\mathrm{NN},\alpha}^{[3]} + \tilde{V}_{\mathrm{3N},\alpha}^{[3]}$, by subtracting one from the other. Again different three-body channels, which are defined by the quantum numbers T_{12}, J_{12}, and π_{12}, can be evolved separately.

Using such a subtraction we have to take additional issues into account, as one has to decide on the truncation in two- and three-body space. For all matrix elements that are produced for use in a many-body calculation we employ a simple scheme, where the energy truncation of matrix elements evolved in two-body space is identical to the truncation of the matrix elements they are subtracted from. The energy truncation then only depends on the three-body channel in question, where we use lower energy truncations for channels with a higher angular momentum, introducing an 'energy ramp':

$$E_{\mathrm{max}}^{\mathrm{SRG},2} = E_{\mathrm{max}}^{\mathrm{SRG},3} = \begin{cases} 40 & \text{if } J_{12} \leq \frac{5}{2} \\ 36 & \text{if } J_{12} = \frac{7}{2} \\ 32 & \text{if } J_{12} = \frac{9}{2} \\ 28 & \text{if } J_{12} = \frac{11}{2} \\ 24 & \text{if } J_{12} \geq \frac{13}{2} \end{cases} \tag{5.24}$$

This subtraction scheme is not entirely consistent, as the irreducible two-body parts evolved in two-body space might be different from the irreducible two-body parts obtained with a SRG transformation in three-body space. For example, a channel with negative parity and an energy limit of $E_{\mathrm{max}}^{\mathrm{SRG},3} = 40$ actually has an energy limit of 39, as matrix elements with $E_{12} = 40$ have positive parity. Nonetheless, for the subtraction scheme we use irreducible two-body parts that haven been transformed in a two-body model space with an energy limit of $E_{\mathrm{max}}^{\mathrm{SRG},2} = 40$. However, for sufficiently large $E_{\mathrm{max}}^{\mathrm{SRG},3}$ it yields correct results.

When producing three-body matrix elements for a subtraction scheme to get irreducible four-body matrix elements, the energy limit is usually lower and, therefore, we have to be more careful about subtraction schemes. In that case there are multiple other possibilities, which are discussed in the next section.



(a) $\alpha = 0.00\text{fm}^4$ **(b)** $\alpha = 0.04\text{fm}^4$

(c) $\alpha = 0.08\text{fm}^4$ **(d)** $\alpha = 0.16\text{fm}^4$

Figure 5.1: The figure shows the absolute value of the NN+3N interaction matrix elements in the four-body Jacobi basis. The matrix elements of the $J^{\pi_{123}}_{123} = 0^+$, $T_{123} = 0$ channel are shown for different values of α. The HO basis is defined with a frequency of $\hbar\omega = 24$ MeV and the SRG evolution is performed in a model space with a truncation of $E^{\text{SRG},4}_{\text{max}} = 16$. The figure has been provided by A. Calci (personal communication, 2013).

5.2.3 Four-Body Part

For the transformation in four-body space, we use the four-body Jacobi basis,

$$\left|E_{123} i_{123} J_{123} T_{123}\right\rangle_a , \tag{5.25}$$

which has been discussed in detail in Sec. 4.1.4, using the following truncation:

$$E_{123} \leq E^{\text{SRG},4}_{\text{max}}. \tag{5.26}$$

Again the channels can be evolved separately, where a channel is defined by T_{123}, J_{123} and π_{123}.

In Fig. 5.1 the evolution in four-body space for one channel is shown. The figure depicts the absolute values of the matrix elements in four-body Jacobi basis. For larger α values, the off-diagonal matrix elements diminish as expected.

The subtraction scheme is more involved than the one for the three-body case. We have to subtract irreducible two- and three-body parts. To achieve that, we need the results of the SRG transformations in two-, three- and four-body space. The kinetic energy is subtracted from all of them. We then have irreducible two-body parts from

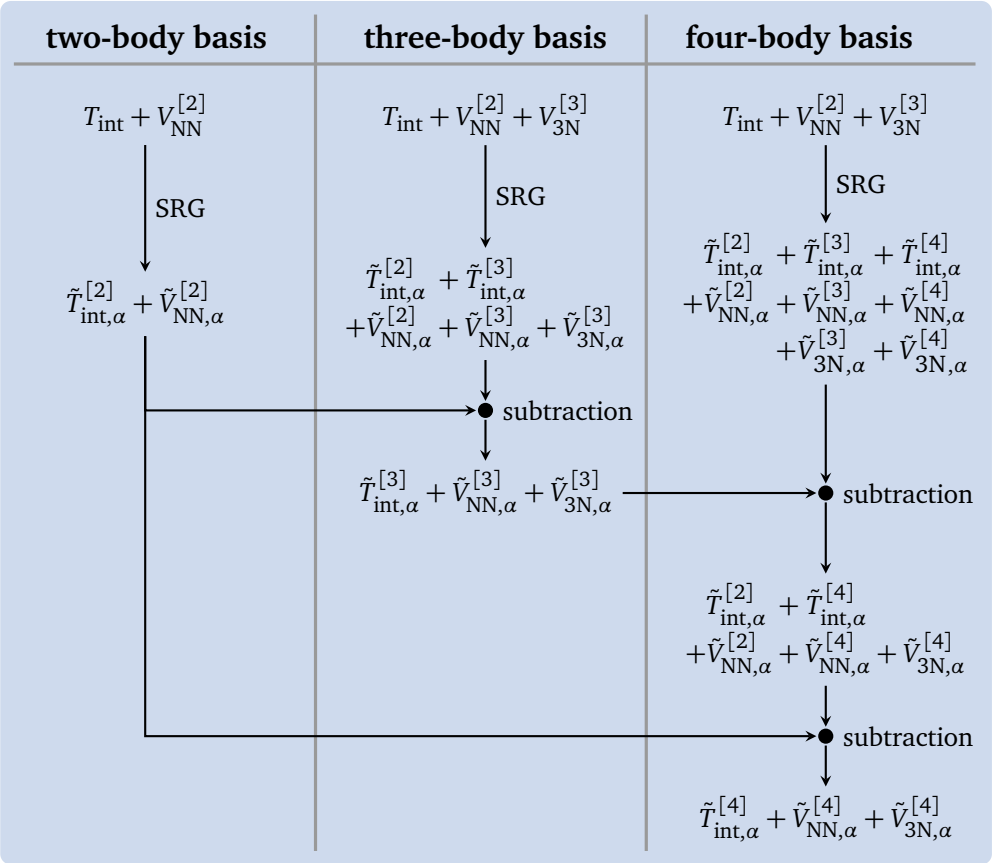


Figure 5.2: Subtraction scheme for getting the irreducible four-body interaction out of a SRG transformation. Note that the initial intrinsic kinetic energy is subtracted directly after each SRG transformation, which is not shown in this figure for brevity.

the transformation in two-body space. Those are subtracted from the evolved interaction in three- and in four-body space. That yields irreducible three-body parts, which are then subtracted from the former result in four-body space. The approach yields irreducible four-body parts and it is illustrated in Fig. 5.2.

Furthermore, we still have multiple possibilities regarding the truncations in the three different spaces, which are discussed in this section. Note that all of the following schemes would yield the same result for an infinite energy limit. For an energy truncation that is large enough, results are expected to be similar for all schemes. The schemes differ in the consistency regarding the truncations in two-, three-, and four-body space. While subtraction scheme A is the easiest scheme using one truncation for all SRG transformations, it has multiple issues. We successively handle these issues in subtraction schemes B, C and D. In the case of scheme D, the energy truncation for the SRG evolution always corresponds to the energies necessary for the different subtractions.

subtraction scheme A

The subtraction scheme A is a straightforward extension from the three-body case. All three truncations are identical:

$$E_{\text{max}}^{\text{SRG},2} = E_{\text{max}}^{\text{SRG},3} = E_{\text{max}}^{\text{SRG},4}. \tag{5.27}$$

This scheme is simple and the SRG evolution only needs to performed for one specific energy. However, the mismatch is the same as in the three body case: if the four-body channel has a negative parity and we have an even energy limit, e.g., $E_{\text{max}}^{\text{SRG},4} = 20$, the actual limit is 19 and we still subtract matrix elements that have been transformed in two- or three-body space with an energy limit of 20.

subtraction scheme B

For this scheme, the truncation is chosen depending on the parity of the four-body channel, e.g., a limit of 20/21 stands for

$$E_{\text{max}}^{\text{SRG},2} = E_{\text{max}}^{\text{SRG},3} = E_{\text{max}}^{\text{SRG},4} = \begin{cases} 21 & \text{if } \pi_{123} = -1 \\ 20 & \text{otherwise} \end{cases} \tag{5.28}$$

In the case of scheme A, we could use the same two- and three-body SRG-transformed matrix elements for all four-body channels. For the subtraction scheme B we need to invest more effort, as we need to perform the SRG evolution of two- and three-body parts for two different energies.

subtraction scheme C

The subtraction scheme B still has a mismatch regarding the subtraction of the irreducible two-body forces from the result of the SRG transformation in three-body space. Having a four-body channel with positive parity and an energy limit of 20, we subtract two-body matrix elements that have been evolved with $E_{\text{max}}^{\text{SRG},2} = 20$ from three-body matrix elements. This also applies to three-body channels that have negative parity, which have an effective limit of 19. To account for this, we determine the SRG model space for the two-body space by using the actual energy limit of the channel we want to subtract them from. This only changes the two-body truncation for those matrix elements that are used for the subtraction in three-body space. We still substract the same two-body matrix elements from the evolved four-body ones as in the case of scheme B:

$$E_{\text{max}}^{\text{SRG},3} = E_{\text{max}}^{\text{SRG},4} = \begin{cases} 21 & \text{if } \pi_{123} = -1 \\ 20 & \text{otherwise} \end{cases} \tag{5.29}$$

$$E_{\text{max}}^{\text{SRG},2} = \begin{cases} 21 & \text{if } \pi_{12} = -1 \text{ and } E_{\text{max}}^{\text{SRG},3} = 21 \\ 19 & \text{if } \pi_{12} = -1 \text{ and } E_{\text{max}}^{\text{SRG},3} = 20 \\ 20 & \text{if } \pi_{12} = +1 \end{cases} \Bigg\} \text{ subtracting two-body from three-body contributions}$$
$$\Bigg\{ \begin{cases} 21 & \text{if } \pi_{123} = -1 \\ 20 & \text{if } \pi_{123} = +1 \end{cases} \text{ subtracting two-body from four-body contributions} \tag{5.30}$$

which we would name $E_{\text{max}}^{\text{SRG},4} = 20/21$.

subtraction scheme D

The difference between the scheme D and the scheme C lies in the treatment of the two-body part that is subtracted from the evolved four-body channel. In the scheme C, the energy limit of the two-body SRG evolution depends on the parity of the four-body channel. However, the two-body parts that are subtracted from the three-body ones depend on the parity of the three-body channel. We want to apply the same treatment for both cases, representing the two-body interaction in three-body space before subtracting it from the four-body channel. For transforming three-body matrix elements of an irreducible two-body contribution to four-body space, we have to be careful about the factors, as discussed in Sec. 4.6 In this case the same two-body space energy limits $E_{\text{max}}^{\text{SRG},2}$ are used for both, subtraction from three- and four-body channels:

$$E_{\text{max}}^{\text{SRG},3} = E_{\text{max}}^{\text{SRG},4} = \begin{cases} 21 & \text{if } \pi_{123} = -1 \\ 20 & \text{otherwise} \end{cases} \tag{5.31}$$

$$E_{\text{max}}^{\text{SRG},2} = \begin{cases} 21 & \text{if } \pi_{12} = -1 \text{ and } E_{\text{max}}^{\text{SRG},3} = 21 \\ 19 & \text{if } \pi_{12} = -1 \text{ and } E_{\text{max}}^{\text{SRG},3} = 20 \\ 20 & \text{if } \pi_{12} = +1 \end{cases} \tag{5.32}$$

which we denote by $E_{\text{max}}^{\text{SRG},4} = 20/21$.

6 Many-Body Calculation

After the SRG transformation of the initial χEFT interaction and the subsequent transformation to the JT-coupled scheme, we want to solve the stationary Schrödinger equation,

$$H\left|\psi_i\right\rangle = E_i\left|\psi_i\right\rangle, \tag{6.1}$$

for a given nucleus, where we are interested in the eigenvalues E_i. We only focus on the lowest eigenvalue, the ground-state energy, which we use to investigate our new interactions that include irreducible four-body parts from the SRG evolution.

An completely exact calculation would in principle require an infinite model space, and is therefore not possible. However, our many-body methods, i.e., the NCSM and IT-NCSM, converge to the exact results when increasing the model space size. Therefore, the calculation can be performed for any desired accuracy, as long as the model space stays small enough to handle it. For simplicity we first discuss the no-core shell model (NCSM) without any importance truncation.

The most prominent feature of the NCSM is its model space. It uses antisymmetric HO states for building the model space. In principal, different kinds of HO bases are possible, but we focus on the m-scheme (Sec. 4.2), i.e., Slater-determinants of single-particle HO states. First, the possible unperturbed Slater determinants are constructed, i.e., all m-scheme basis states with the lowest HO energy possible are included. For example, ^{4}He would have two protons and two neutrons in the s-shell. The total HO energy quantum number is $E = 0$ in this case and there is only one Slater determinant that can be constructed. In the case of ^{5}He, an additional neutron can be found in the p-shell, raising the total HO energy quantum number to $E = 1$. Since we have multiple single-particle states in the p-shell with the same HO energy, we have to add all the possible Slater determinants to our model space that have one neutron in one of the p-shell single-particle states while the other two neutrons occupy the s-shell.

In a second step, excited HO configurations are added. We find these configurations by taking one of the unperturbed Slater determinants and moving one or multiple nucleons to states in upper shells. The relevant parameter in this case is the excitation energy: As the energy difference between adjacent shells is always $\hbar\omega$, we simply count the total number of shells we lift the particles. For example, Fig. 6.1 shows a 6 $\hbar\omega$ configuration for ^{16}O. This number is limited by $N_{\max}$, e.g., a model space with $N_{\max} = 2$ includes all the unperturbed Slater determinants, all configurations where one particle has been lifted one or two shells and all configurations where two particles have been lifted one shell each.

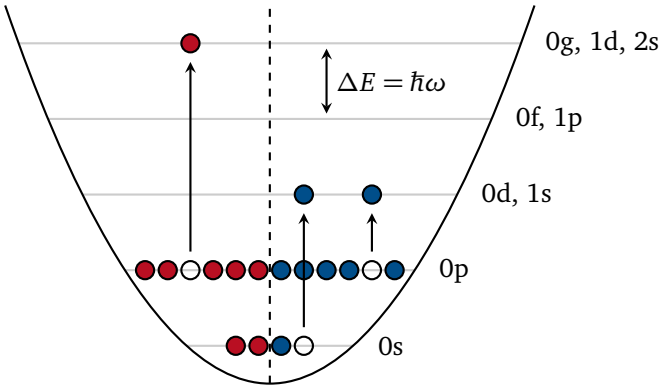


Figure 6.1: Configuration for ^{16}O with an excitation energy of 5 $\hbar\omega$. Neutrons are depicted as blue dots, whereas protons are red.

For a given nucleus and $N_{\max}$ truncation, we can construct the necessary energy truncation $E^4_{\max}$, which we use for the four-body m-scheme representations of the interaction. For instance, a consistent $N_{\max} = 2$ calculation of ^{4}He needs four-body m-scheme matrix elements with $E^4_{\max} = 2$. An ^{16}O calculation, on the other hand, would require matrix elements with $E^4_{\max} = 6$, as picking four particles out of a 16-body NCSM model space with $N_{\max} = 2$ can at most yield a total HO energy quantum number of $E = 6$ for these four particles.

Once we have the model space set up, the matrix elements must be calculated. As we already know how to convert interactions that are represented in the Jacobi basis to the two-, three- or four-body m-scheme, we can simply use the previously derived rules (see Sec. 4.6.1) to calculate the interaction matrix in the many-body m-scheme basis relevant for the nucleus. Once that is done, the matrix can be diagonalized, which yields eigenvalues and eigenstates.

These calculations are done with different values for $N_{\max}$. If it could be increased to infinity, we would encounter the exact solution. However, even for finite values the calculation yield results that are close to the exact energy. If convergence cannot be reached by increasing $N_{\max}$, it is still possible to extrapolate the results to higher values. Furthermore the variational principle holds for NCSM calculations: They always yield an upper limit and can never be lower than the exact value. These two principles lead to the typical representation of NCSM results, which is a monotonic decrease of the energy eigenvalues with increasing $N_{\max}$, where the values converge towards the exact result for an appropriate basis like the HO basis.

6.1 Importance Truncation

The NCSM model space dimension increases rapidly with the number of nucleons and the truncation $N_{\max}$. Therefore, convergence with respect to $N_{\max}$ can only be achieved for s- and p-shell nuclei. However, the calculations can be extended to sd-shell nuclei by introducing an importance truncation. It attacks the problem of large matrices by neglecting configurations that are not relevant or 'important' for the calculation. This yields a new, smaller model space, which results in smaller matrices.

When applying this truncation, we have to decide on a target state that we would like to calculate, e.g., the ground state. For selecting relevant configurations we can then define an importance measure, κ_i, for every possible configuration $\left|\Psi_i\right\rangle$:

$$\kappa_i = \frac{\left\langle \Psi_i \right| H \left| \psi_{\text{ref}} \right\rangle}{\epsilon_{\text{ref}} - \epsilon_i}, \tag{6.2}$$

where $\left|\Psi_{\text{ref}}\right\rangle$ is a reference state that should approximate the target state. Such an approximation can, for example, be obtained by a NCSM calculation with a low $N_{\max}$ truncation. For a subsequent IT-NCSM calculation only basis states with an importance measure greater than some specific threshold, $|\kappa_i| > \kappa_{\min}$, are considered. For a threshold of $\kappa_{\min} = 0$ the IT-NCSM corresponds to the original NCSM. Equation (6.2) is based on multiconfigurational perturbation theory, it corresponds to the amplitude of the state $\left|\Psi_i\right\rangle$ in the first-order correction to the reference-state.

We also have to calculate the energies ϵ_{ref} and ϵ_i. One possible choice would be expectation values,

$$\epsilon_{\text{ref}} = \left\langle \Psi_{\text{ref}} \right| H \left| \Psi_{\text{ref}} \right\rangle \tag{6.3}$$

$$\epsilon_i = \left\langle \Psi_i \right| H \left| \Psi_i \right\rangle, \tag{6.4}$$

which is known as Epstein-Nesbet partitioning. Instead, we will use the simpler Møller-Plesset partitioning, where the difference between the energies,

$$\Delta\epsilon = \epsilon_{\text{ref}} - \epsilon_i, \tag{6.5}$$

is given by the excitation energy of the the configuration $\left|\Psi_i\right\rangle$. This choice avoids the additional time needed to compute the expectation values.

In practice we will apply the IT-NCSM iteratively: We decide on a target state and an importance threshold. We first start with a $N_{\max} = 4$ NCSM calculation, resulting in a reference state. Afterwards an importance-truncated model space $\mathcal{M}_6$, is constructed by using a $N_{\max} = 6$ model space and truncating it to the 'important' configurations as described above. In that space an IT-NCSM calculation is done, yielding a new reference state. With that reference state a new model space $\mathcal{M}_8$, based on a $N_{\max} = 8$ model space, is constructed. This scheme is repeated until a sufficiently large $N_{\max}$ is reached.

Nonetheless, the importance threshold does influence the results. To obtain the original NCSM result, the importance-truncation scheme is applied for different values of $\kappa_{\min}$. Afterwards we can extrapolate the results to $\kappa_{\min} = 0$. A detailed description of the importance truncation and its application to the NCSM has been given by Roth [35].

7 Results

In this chapter we discuss the results obtained from (IT-)NCSM calculations using SRG transformed interactions from χEFT. Special attention is paid to the effect of the irreducible four-body forces that have been induced during the SRG evolution. We mainly check our methods by calculating ground-state energies of ^{16}O for different parameters, i.e., different subtraction schemes, frequencies $\hbar\omega$, α values, and $N_{\max}$, as oxygen shows a dependence on α without four-body forces [14]. Therefore, we expect the four-body forces to become increasingly repulsive for larger values of α to reduce this dependence. As few-body basis states with low angular momentum are usually the most important ones for low-energetic many-body configurations, we will restrict the investigations to the lowest four-body angular momenta. Furthermore, calculations with ^{6}Li are performed, which is almost independent of α without four-body forces [14]. Therefore, we expect four-body forces not to influence its ground-state energy, providing a check for the induced four-body forces included in our interaction.

The interactions used in the many-body calculations differ in the truncation of the particle number, the initial interactions and the methods employed for induced four-body forces. We, therefore, use the following notation to discern between them:

- **NN-only** — SRG-evolved initial two-body interaction omitting any induced three- or four-body parts.
- **NN+3N-induced** — SRG-evolved initial two-body interaction including induced three-body parts and omitting four-body ones.
- **NN+3N-induced+4N-induced** — SRG-evolved initial two-body interaction including induced three- and four-body parts.
- **NN+3N-full** — SRG-evolved initial two- and three-body interaction omitting induced four-body parts.
- **NN+3N-full+4N-induced** — SRG-evolved initial two- and three-body interaction including induced four-body parts.
- **NN+3N-full+4N-sum** — SRG-evolved initial two- and three-body interaction. The induced four-body part is summed over yielding an effective three-body interaction (see Sec. 4.5).

As the four-body forces are diagonal in angular momentum, parity, and isospin, we define a four-body channel in Jacobi basis by the quantum numbers J_{123}, π_{123}, and T_{123}. We distinguish between included four-body channels, when using an interaction that includes induced four-body forces (NN+3N-induced+4N-induced, NN+3N-full+4N-induced or NN+3N-full + 4N-sum). They are always added in the same order: The first included channel is the helium-channel with $J_{123} = 0$, $T_{123} = 0$ and $\pi_{123} = +1$. Then the negative parity channel $\pi_{123} = -1$ is added. Afterwards channels with higher isospin are included. Having included all six channels with $J_{123} = 0$, we raise the angular momentum to $J_{123} \leq 1$ and $J_{123} \leq 2$. The following table shows the order of inclusion and numbers the different partial waves (PW). From here on, these numbers will be used as an abbreviation for the included PWs.

PW	included four-body $J^\pi T$ channels
0	no induced four-body channels
1	0^+0
2	$0^\pm0$
3	$0^\pm0$, 0^+1
4	$0^\pm0$, $0^\pm1$
5	$0^\pm0$, $0^\pm1$, 0^+2
6	$0^\pm0$, $0^\pm1$, $0^\pm2$
7	$0^\pm0$, $0^\pm1$, $0^\pm2$, 1^+0
8	$0^\pm0$, $0^\pm1$, $0^\pm2$, $1^\pm0$
9	$0^\pm0$, $0^\pm1$, $0^\pm2$, $1^\pm0$, 1^+1
10	$0^\pm0$, $0^\pm1$, $0^\pm2$, $1^\pm0$, $1^\pm1$
11	$0^\pm0$, $0^\pm1$, $0^\pm2$, $1^\pm0$, $1^\pm1$, 1^+2
12	$0^\pm0$, $0^\pm1$, $0^\pm2$, $1^\pm0$, $1^\pm1$, $1^\pm2$
13	$0^\pm0$, $0^\pm1$, $0^\pm2$, $1^\pm0$, $1^\pm1$, $1^\pm2$, 2^+0
14	$0^\pm0$, $0^\pm1$, $0^\pm2$, $1^\pm0$, $1^\pm1$, $1^\pm2$, $2^\pm0$
15	$0^\pm0$, $0^\pm1$, $0^\pm2$, $1^\pm0$, $1^\pm1$, $1^\pm2$, $2^\pm0$, 2^+1
16	$0^\pm0$, $0^\pm1$, $0^\pm2$, $1^\pm0$, $1^\pm1$, $1^\pm2$, $2^\pm0$, $2^\pm1$
17	$0^\pm0$, $0^\pm1$, $0^\pm2$, $1^\pm0$, $1^\pm1$, $1^\pm2$, $2^\pm0$, $2^\pm1$, 2^+2
18	$0^\pm0$, $0^\pm1$, $0^\pm2$, $1^\pm0$, $1^\pm1$, $1^\pm2$, $2^\pm0$, $2^\pm1$, $2^\pm2$

When all channels with $J_{123} = 0$ are included, for instance, we would name it PW = 6 and including all channels with $J_{123} \leq 1$ is denoted by PW = 12.

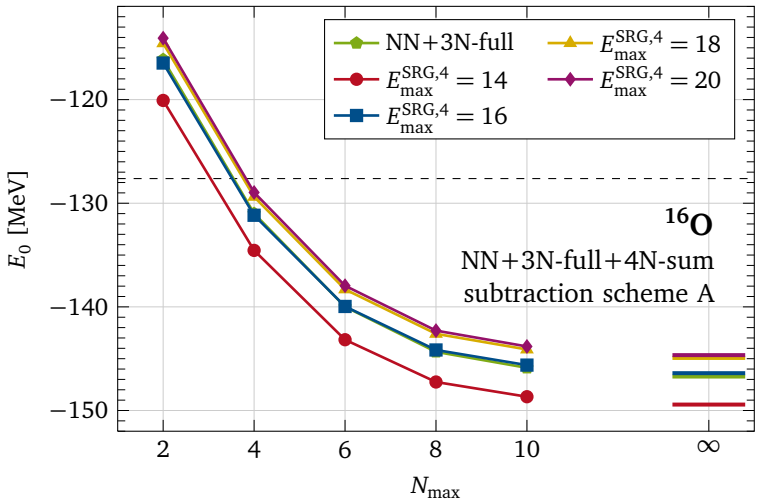


Figure 7.1: ^{16}O ground-state energy over (IT-)NCSM model-space size with NN+3N-full(+4N-sum) interactions. Results for $N_{\max} \leq 4$ are NCSM calculations, all other results were obtained using the IT-NCSM. The values for $N_{\max} \to \infty$ were extrapolated by fitting an exponential function to the three data points at $N_{\max} = 6, 8, 10$. Only the helium channel (PW = 1) was included for the NN+3N-full+4N-sum calculations. Furthermore, $\alpha = 0.08\,\mathrm{fm}^4$ and $\hbar\omega = 24$ MeV was used. The dashed line indicates the experimental value [36].

7.1 Effective Three-Body Interaction

In this section we analyze the results obtained by approximating the induced four-body forces by a three-body force. This partial-trace approximation is designed to be simple and only used for testing the effect of the four-body forces. It is an uncontrolled approximation and the explicit inclusion of four-body forces are the preferred method. For details of the approximation see Sec. 4.5. All the results presented were calculated with the subtraction scheme A.

We first examine the dependence of ^{16}O ground-state energy on the SRG model space using the (IT-)NCSM, which is presented in Fig. 7.1. The results were obtained by using a single four-body channel only, nevertheless they look promising. While the effect of including four-body forces is attractive for small SRG model spaces, the energy increases with $E_{\max}^{\mathrm{SRG},4}$. Additionally, the results for $E_{\max}^{\mathrm{SRG},4} = 18$ and $E_{\max}^{\mathrm{SRG},4} = 20$ seem to be almost identical, indicating a convergence with respect to the SRG model space. Moreover, the convergence with respect to the NCSM model-space size is not affected, the results for the ground-state energy seem to be shifted by the same amount independently of $N_{\max}$.

However, the shift of approximately 2 MeV is not large enough to remove the α dependence competely. Therefore we investigate the effect of additional four-body channels. This is done using the (IT-)NCSM, as presented in Fig. 7.2. Obviously, including additional channels can increase the ground-state energy, which is the expected effect. The influence of the channels seems to vary. While PW = 2 and PW = 3 show small effects only, including the fourth channel increases the energy by 2 MeV.

An (IT-)NCSM calculation that is converged with respect to the SRG and the NCSM model-space sizes and including all relevant four-body channels is expected to yield results for the ^{16}O ground state that are independent of α, which would require stronger repulsive effects than the ones of the included four-body channels discussed above. However, we obtained results by using a simple formula and the existing three-body framework. The calculations only used the first four channels and the formula requires multiple uncontrolled approximations. Nevertheless, the obtained ground-state energies already indicate a repulsive effect of the four-body channels, although it is not strong enough to remove the α dependence. Considering the restrictions on these calculations, an explicit inclusion of the four-body contributions might increase the repulsive effect to the desired strength. Therefore a more thorough investigation is performed by explicitly including four-body forces in the (IT-)NCSM calculations.

7.2 Explicit Four-Body Interaction

In the following sections we discuss results obtained using the induced four-body interaction by transforming it to the JT-coupled scheme. Many of the following calculations investigate the effect of a different number of included channels and effects of the SRG model space truncation. As this investigation implies numerous NCSM calculations, the NCSM model space is reduced to $N_{\max} = 2$ or $N_{\max} = 4$. While these small model spaces entail results that

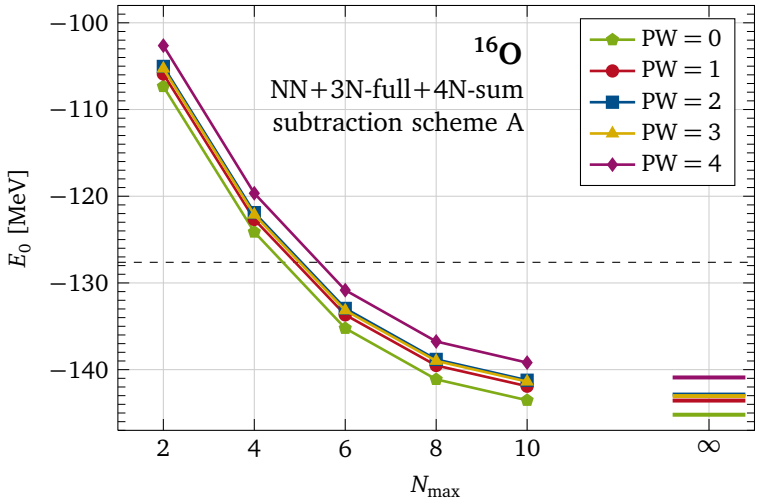


Figure 7.2: ^{16}O ground-state energy over (IT-)NCSM model-space size with NN+3N-full(+4N-sum) interactions. Results for $N_{\max} \leq 4$ are NCSM calculations, all other results were obtained using the IT-NCSM. The values for $N_{\max} \to \infty$ were extrapolated by fitting an exponential function to the three data points at $N_{\max} = 6, 8, 10$. For the NN+3N-full+4N-sum calculations $E_{\max}^{\mathrm{SRG},4} = 20$ was used. Furthermore, $\alpha = 0.0625$ fm^4 and $\hbar\omega = 24$ MeV was used. The dashed line indicates the experimental value [36].

are far from convergence, we expect the differences that we want to analyze to be visible irrespective of the NCSM model space, as the results obtained by the partial trace approximation indicated that the energy shift is more or less independent of $N_{\max}$ (see Sec. 7.1).

Keep in mind that the energy truncation in the JT-coupled scheme is lower than in the Jacobi basis, as it requires more matrix elements to represent the Hamiltonian and, therefore, more storage space is necessary. The truncation of the four-body HO energy quantum number in the four-body JT-coupled scheme is named $E_{\max}^4$. It should not be confused with the truncation of the SRG model space, $E_{\max}^{\mathrm{SRG},4}$, which is a truncation of relative HO energy used for the SRG evolution. For an ^{16}O calculation with $N_{\max} = 2$, $E_{\max}^4 = 6$ is not an approximation, as all possible four-body interactions in the 16-body NCSM basis with $N_{\max} = 2$ can be represented with an HO energy quantum number of $E \leq 6$. This truncation is an approximation for higher $N_{\max}$ only.

7.2.1 Subtraction Schemes

We first analyze the effect of different four-body channels and SRG model-space sizes using the ^{16}O ground-state energy calculations with the subtraction scheme A. The results are presented in Fig. 7.3. Contrarily to the calculations with the partial trace approximation, we see huge differences between the ^{16}O ground-state energies for different values of $E_{\max}^{\mathrm{SRG},4}$. Obviously the SRG transformation is not converged with respect to the SRG model space, which poses a problem for reliable calculations with four-body forces.

Furthermore, we observe a surprising effect regarding the four-body channels: When including all channels with $J_{123} = 0$ (PW = 6), the difference betweeen a $E_{\max}^{\mathrm{SRG},4} = 18$ and a $E_{\max}^{\mathrm{SRG},4} = 14$ calculation is approximately 16 MeV. Including all channels with $J_{123} \leq 1$ (PW = 12), the difference grows to 80 MeV. The convergence for channels with $J_{123} = 1$ seems to be far worse than for $J_{123} = 0$ ones. The repulsive effect, we expected to see, is visible, at least for the larger SRG model spaces. While the difference between PW = 0 and PW = 6 is about 7 MeV for $E_{\max}^{\mathrm{SRG},4} = 18$, the difference between PW = 0 and PW = 12 is approximately 46 MeV. Again, the $J_{123} = 1$ channels seem to have considerably stronger influence than the $J_{123} = 0$ channels.

The slow convergence of the four-body forces can have multiple reasons. As the four-body SRG model space is too small to reflect the important features of the initial two- and three-body forces, the evolution in four-body space yields incomplete two- and three-body forces, which depend strongly on the model-space truncation. This has two effects, on the one hand, incomplete two- and three-body forces induce incomplete four-body forces. This can only be rectified by using larger model spaces. On the other hand, subtracting two- and three-body forces that were evolved with slightly different truncations can have a big impact. Therefore, we have to compare the different subtraction schemes and analyze the convergence with respect to $E_{\max}^{\mathrm{SRG},4}$. As a basis for this analysis NCSM

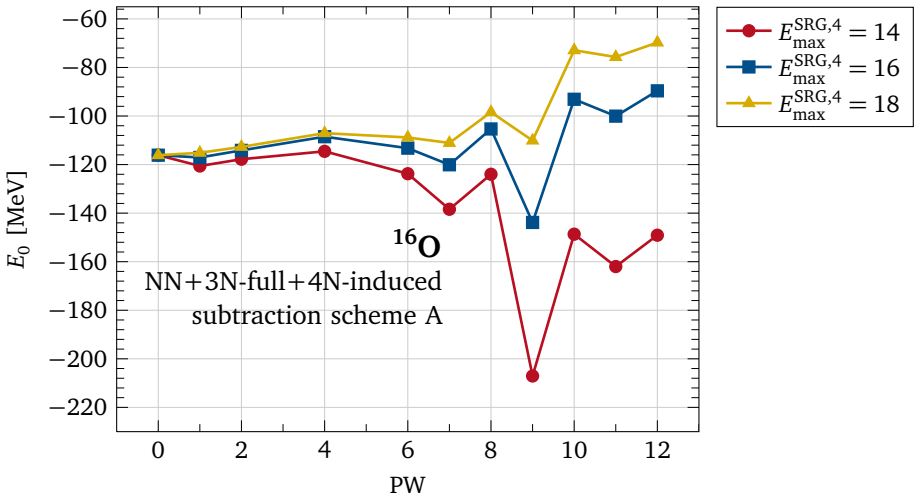


Figure 7.3: NN+3N-full+4N-induced calculations of the ^{16}O ground state over the number of induced four-body channels using subtraction scheme A. Furthermore $\alpha = 0.08$ fm^4, $\hbar\omega = 24$ MeV, $N_{\max} = 2$ and $E_{\max}^4 = 6$ was used.

calculations for ^{16}O have been performed with a small model space $N_{\max} = 2$. The calculations have been done for all four subtraction schemes, different sets of included four-body channels and varying $E_{\max}^{\mathrm{SRG},4}$. The resulting ground-state energies are summarized inFig. 7.4.

Considering different $E_{\max}^{\mathrm{SRG},4}$ truncations and the influence of different partial waves, we find similar features for results obtained with different subtraction schemes. None of the subtraction schemes seems to be converged with respect to $E_{\max}^{\mathrm{SRG},4}$ and the convergence becomes worse for higher J_{123} channels. For including channels with $J_{123} > 1$ we require model spaces with $E_{\max}^{\mathrm{SRG},4} > 20$, which is computationally too demanding at present. Repulsive effects seem to be present for high $E_{\max}^{\mathrm{SRG},4}$ values in all schemes, where the $J_{123} = 1$ channels have a larger influence than the $J_{123} = 0$ ones. Nonetheless, all four subtraction schemes yield different results. While the four-body forces seem to become less repulsive with a larger model space in subtraction scheme C, it is the other way round in the other schemes. Subtraction scheme D does not even converge monotonically. Using $E_{\max}^{\mathrm{SRG},4} = 20$, the subtraction schemes B, C, and D yield results between -109 and -113 MeV for PW $= 6$. For PW $= 12$ the subtraction schemes C and D yield approximately -101 MeV and -92 MeV respectively. These results illustrate the huge differences between subtraction schemes if we handle results that are not converged with respect to $E_{\max}^{\mathrm{SRG},4}$ and make it clear that a subtraction scheme should be chosen with care.

The difference between the subtraction schemes B, C, and D is particularly interesting, as these schemes only differ in the subtraction of two-body forces. Provided that the SRG model space is large enough, the two-body forces do not induce any sizable four-body contributions [14]. In contrast, the effect of two-body forces is clearly visible in our case. A further investigation with a NN+3N-induced+4N-induced is presented in Fig. 7.5. Using only initial two-body forces allows us to gauge the effect of the two-body force on the convergence of the induced four-body force with respect to $E_{\max}^{\mathrm{SRG},4}$. In this case we still observe a slower convergence with increasing PW. For the largest model space, the overall effect of the induced four-body forces on the ground-state energy seems to be strongly repulsive when including all $J_{123} \leq 1$ channels and omitting the initial three-body force. Nevertheless, we expect the four-body forces induced by the initial two-body force to have negligible effects on the total energy for sufficiently large SRG model spaces, if all relevant four-body channels are included. In the case of the NN+3N-induced+4N-induced calculations, however, no convergence with respect to $E_{\max}^{\mathrm{SRG},4}$ has been reached and we cannot include any channels with a higher angular momentum yet. As long as these two issues cannot be solved, we can expect the four-body forces that are induced by the initial two-body forces to have a strong effect. For instance, the energy difference of the ^{16}O ground state between $E_{\max}^{\mathrm{SRG},4} = 20$ and $E_{\max}^{\mathrm{SRG},4} = 14$ for a calculation with the NN+3N-induced+4N-induced interaction with PW $= 12$ is approximately 24 MeV, for the NN+3N-full+4N-induced calculation with the same parameters it is about 11 MeV. Therefore, the initial two-body forces seem to be the reason for the convergence issues with respect to $E_{\max}^{\mathrm{SRG},4}$. In this case the inclusion of initial three-body forces even seems to improve the convergence, indicating that the initial three-body forces play a sizable role as well.

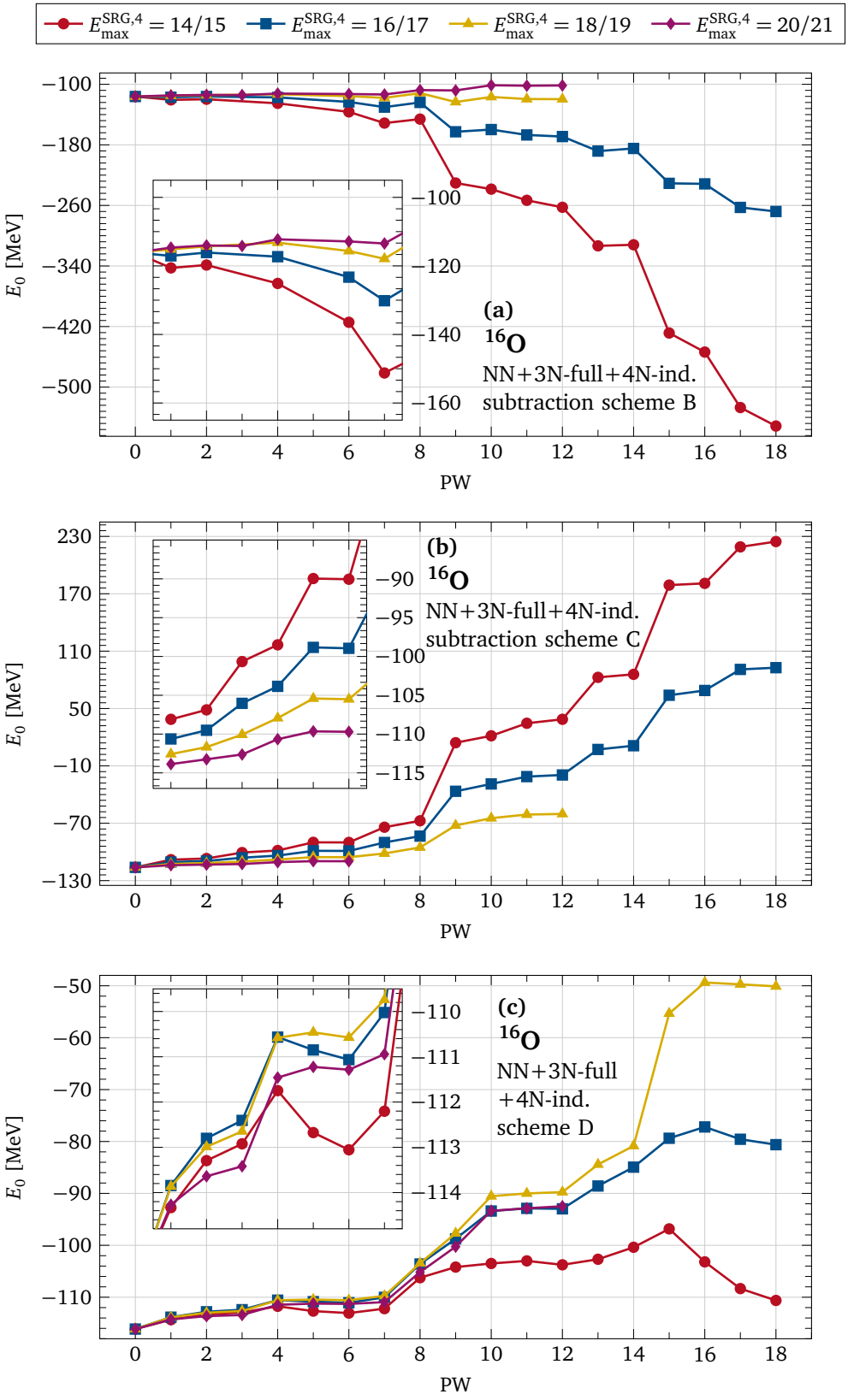


Figure 7.4: Comparison of different subtraction schemes using NN+3N-full+4N-induced interactions. The ^{16}O ground-state energy is plotted over the number of included four-body channels. Furthermore, $\alpha = 0.08\ \mathrm{fm}^4$, $\hbar\omega = 24$ MeV, $N_{\max} = 2$ and $E_{\max}^4 = 6$ were used. Keep in mind that the value for PW = 0 is the same for all figures.

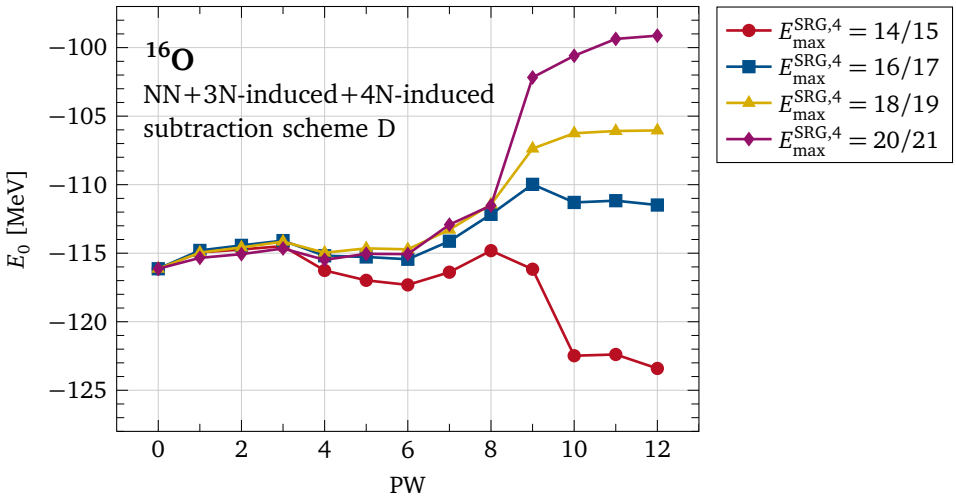


Figure 7.5: The ^{16}O ground-state energy, calculated with NN+3N-induced+4N-induced interactions using subtraction scheme D, is plotted over the number of included four-body channels. Furthermore, $\alpha = 0.08$ fm^4, $\hbar\omega = 24$ MeV, $N_{\max} = 2$ and $E_{\max}^4 = 6$ were used.

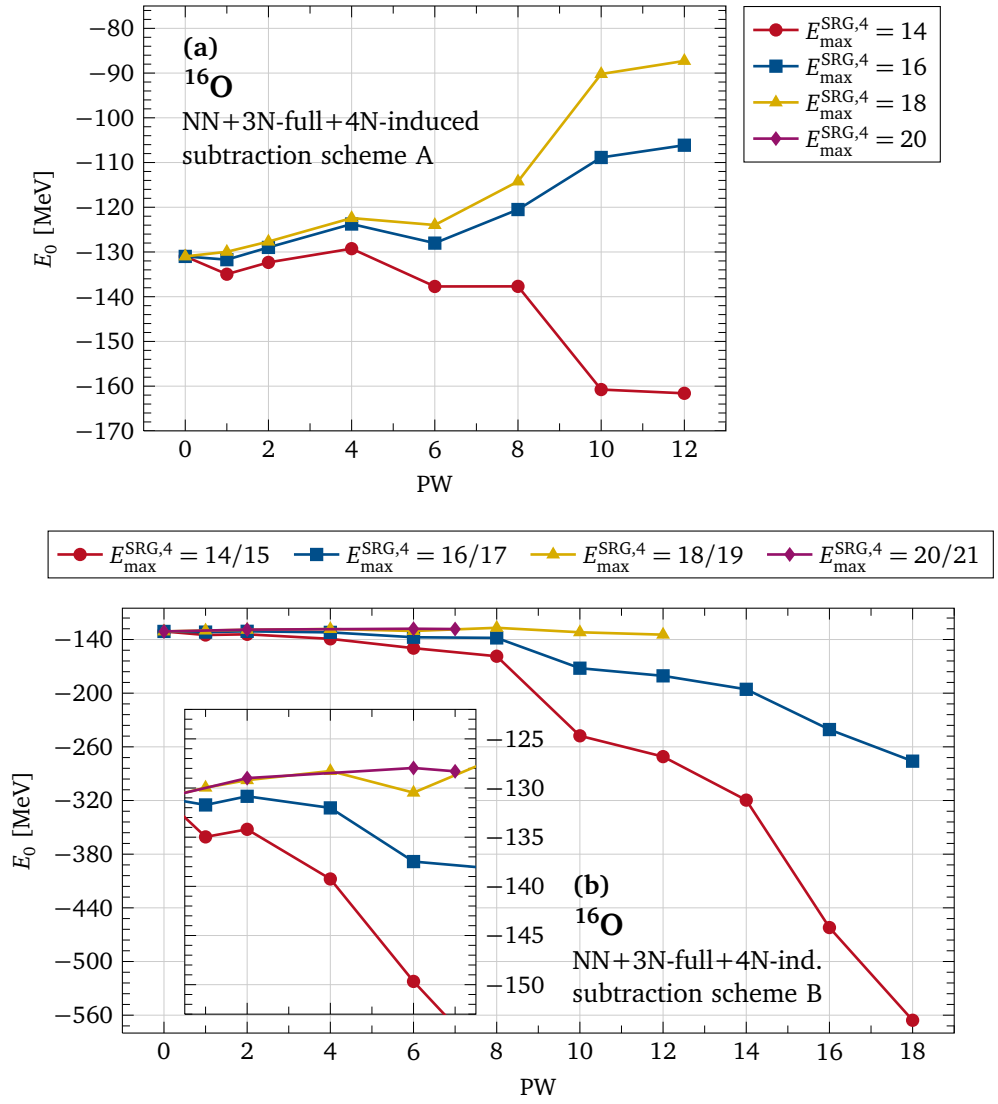


Figure 7.6: Comparison of subtraction schemes A and B using NN+3N-full+4N-induced interactions. The ^{16}O ground-state energy is plotted over the number of included four-body channels. Furthermore, $\alpha = 0.08$ fm^4, $\hbar\omega = 24$ MeV, $N_{\max} = 4$ and $E_{\max}^4 = 6$ were used. Keep in mind that the value for PW = 0 is the same for both figures.

To ensure that the described effects are not an anomaly of the $N_{\max} = 2$ calculations, a few calculations for $N_{\max} = 4$ have been done, which can be found in Fig. 7.6. The results for the ^{16}O ground-state energy show qualitatively the same behavior as for $N_{\max} = 2$. Of course, a higher NCSM model space ensures lower ground-state energies. However, the energy shift between $N_{\max} = 2$ and $N_{\max} = 4$ calculations seems to be mostly independent of the SRG model space truncation or the number of four-body channels. This also confirms the observation from the NN+3N-full+4N-sum calculations, the four-body forces do not influence the convergence behavior with respect to the NCSM model space.

In the following sections we concentrate on the subtraction scheme D, as it is the most consistent scheme (Sec. 5.2.3).

7.2.2 Lithium

For a few parameter combinations, benchmarking calculations have been done for the ^{6}Li ground state. They can be found in Fig. 7.7. As ^{6}Li does not show an dependence on α in NN+3N-full calculations, it is well suited for testing the four-body interactions. While the induced four-body force should remove the α dependence of the NN+3N-full calculation of ^{16}O, the four-body force should have a negligible effect on ^{6}Li.

All calculations show a qualitatively similar behavior to the ^{16}O case: No convergence with respect to the SRG model-space size can be seen, especially when including channels with a higher angular momentum. Furthermore, we find a stronger effect for higher angular momentum. Different values for $\hbar\omega$ or different subtraction schemes change the convergence behavior completely, similar to the ^{16}O calculations. seems to exhibit a monotonic convergence with respect to the SRG model-space size.

However, the scale is different: The difference between a NN+3N-full and a NN+3N-full+4N-induced calculation including all channels with $J_{123} \leq 2$ is at most 2 MeV. For larger SRG model spaces these differences seem to become even smaller. As the ground-state energy of ^{6}Li shows only negligible dependence on α [14], a sizable influence of induced four-body forces has not been expected in the first place. This indicates that even the induced four-body forces that are not converged with respect to $E_{\max}^{\mathrm{SRG},4}$ mainly influence calculations of nuclei showing an α dependence without them. Of course, further tests with other nuclei are necessary to conclusively proove that these induced four-body forces, which are not converged, do not degrade calculations which already show good results at the three-body level. Independent of these investigations we expect induced four-body forces that are converged with respect to $E_{\max}^{\mathrm{SRG},4}$ to have negligible effects on the ground-state energy of ^{6}Li.

7.2.3 Frequency Dependence

Another important factor for any NCSM calculation is the value of $\hbar\omega$, which has a strong influence on convergence with respect to the NCSM model space. In Fig. 7.8 the results for ^{16}O, $N_{\max} = 2$ calculations using three different frequencies are presented. The results for $\hbar\omega = 24$ MeV can be found in Fig. 7.4(c).

On the one hand, $\hbar\omega = 20$ MeV seems to be the best choice for a NN+3N-full calculation, as it yields the lowest ground-state energy, offering the best convergence with respect to $N_{\max}$. On the other hand, the frequency has a huge impact on the induced four-body forces and their convergence behavior with respect to the SRG model-space size. At $\hbar\omega = 20$ MeV the induced forces become more repulsive with higher $E_{\max}^{\mathrm{SRG},4}$, $\hbar\omega = 32$ MeV the induced forces become more attractive for increasing SRG-model space size. For $\hbar\omega = 24$ MeV and $\hbar\omega = 28$ MeV, the changes with SRG model-space size are not even monotonic.

As higher $\hbar\omega$ values have a negative effect on the convergence with respect to the NCSM model space, we will focus on $\hbar\omega = 24$ MeV in the following sections. The frequency was chosen for its good convergence with respect to NCSM model-space size. Furthermore, the convergence with respect to the SRG model space size is not worse than for for other frequencies. We omit $\hbar\omega = 20$ MeV because of its slow convergence with respect to $E_{\max}^{\mathrm{SRG},4}$, e.g., the energy difference of the ^{16}O between $E_{\max}^{\mathrm{SRG},4} = 16$ and $E_{\max}^{\mathrm{SRG},4} = 18$ for PW = 12 is about 8 MeV at $\hbar\omega = 20$ MeV while it is only 3 MeV at $\hbar\omega = 24$ MeV.

We should keep in mind that the difference between ground-state energies for $E_{\max}^{\mathrm{SRG},4} = 20$ and $E_{\max}^{\mathrm{SRG},4} = 18$ in a calculation with PW = 12, subtraction scheme D and $\hbar\omega = 24$ MeV is approximately 3 MeV. Furthermore, the non-monotonic convergence makes it difficult to estimate errors. On top of that, we neglect all channels with $J_{123} \geq 2$, whose effects we cannot even estimate. Therefore, we cannot expect to obtain an accurate result using these parameters. Nevertheless, we might be able to reduce the α-dependence of the ^{16}O NN+3N-full calculations.

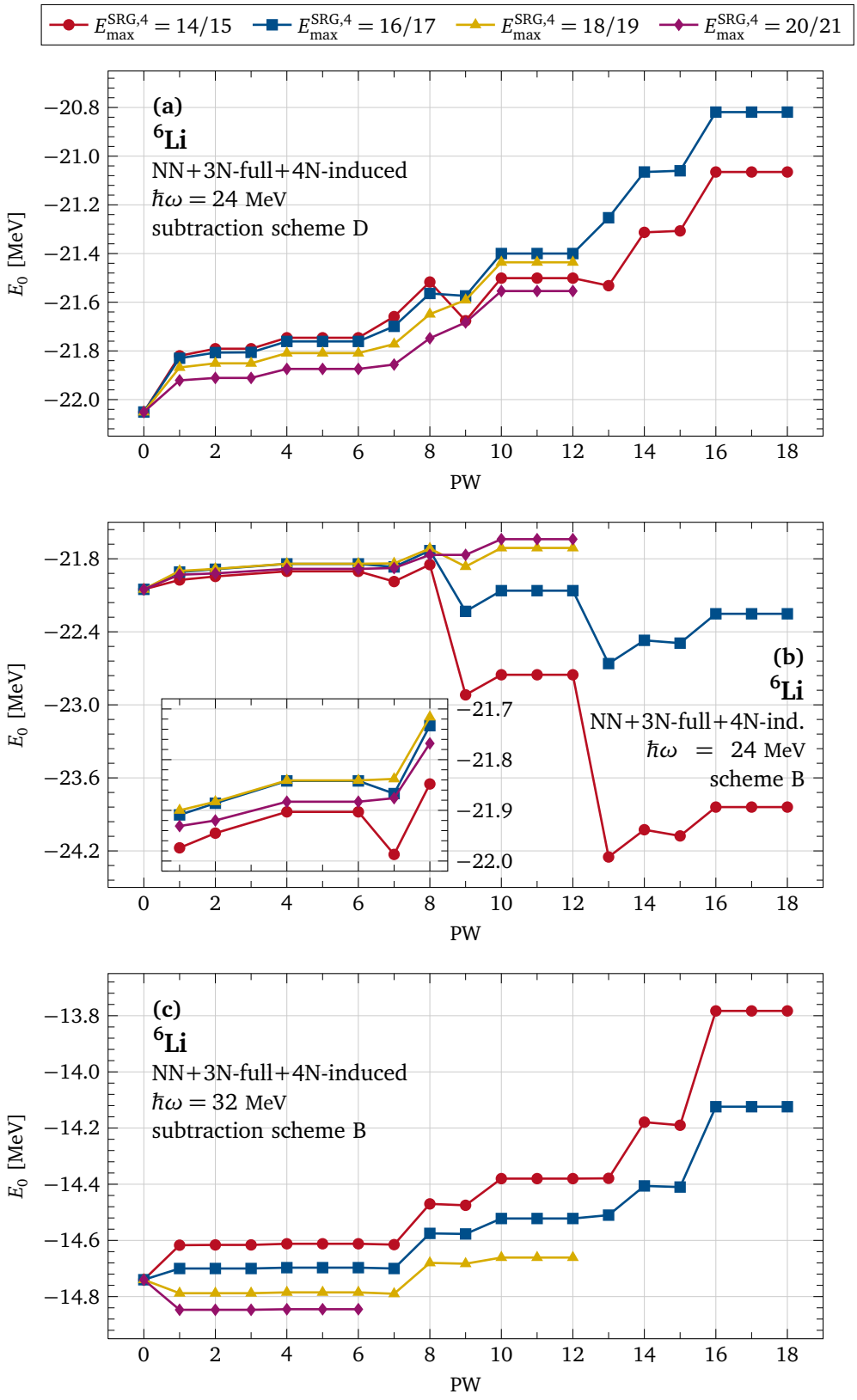


Figure 7.7: Comparison of different parameter combinations using NN+3N-full+4N-induced interactions. The ^{6}Li ground-state energy energy is plotted over the number of included four-body channels. Furthermore, we use $\alpha = 0.08$ fm^4, $N_{\max} = 2$ and $E_{\max}^4 = 6$. The ground state of ^{6}Li has a total isospin of 0, including four-body channels with $T_{123} = 2$ (PW $= 5, 6, 11, 12, 17, 18$) does not influence the energy.

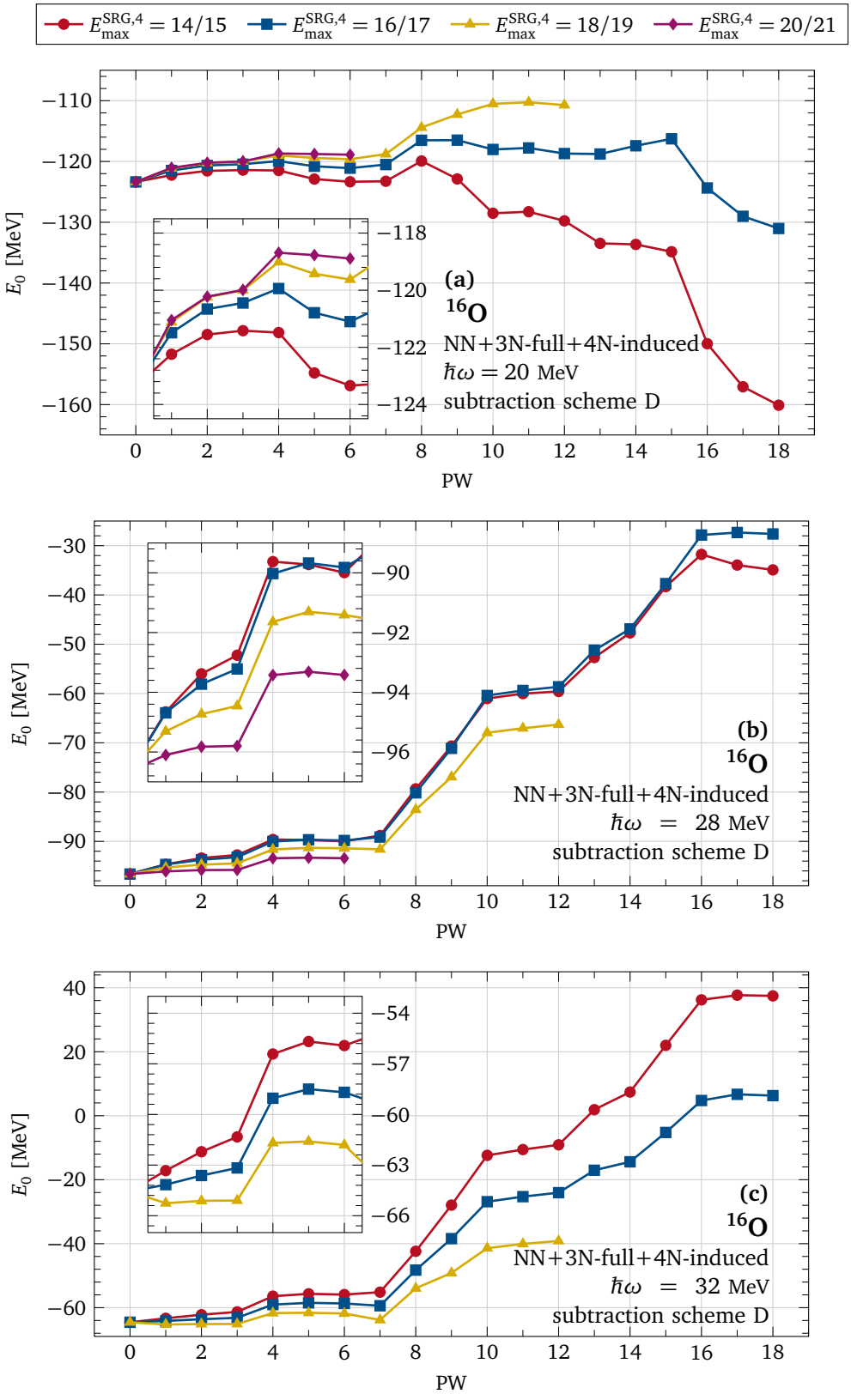


Figure 7.8: Comparison of different $\hbar\omega$ values using NN+3N-full+4N-induced interactions. The ^{16}O ground-state energy is plotted over the number of included four-body channels. Furthermore, $\alpha = 0.08$ fm^4, $N_{\max} = 2$, $E_{\max}^4 = 6$ and subtraction scheme D were used. The corresponding $\hbar\omega = 24$ MeV calculations can be found in Fig. 7.4(c)

7.2.4 α Dependence

Having selected a frequency ($\hbar\omega = 24$ MeV) and a subtraction scheme (D), we can now investigate the effect of the induced four-body forces on the α dependence of the ^{16}O ground-state energy. Calculations for different α-values are presented in Fig. 7.9. As a large value for α should enhance convergence with respect to $N_{\max}$, the energies should generally become lower with increasing α. This can be seen in Fig. 7.9, e.g., the NN+3N-full calculations (PW = 0) yield lower values for the ground-state energy with increasing α. However, we are interested in the α dependence of the ^{16}O ground-state energy for results that are converged with respect to $N_{\max}$. We are, therefore, interested in the difference of the energies between the NN+3N-full and the NN+3N-full+4N-induced calculations, as we expect the difference to be mostly independent of $N_{\max}$. As the converged ^{16}O ground-state energy is lowered with increasing α in an NN+3N-full calculation, the energy difference between the NN+3N-full and the NN+3N-full+4N-induced calculations should increase to mitigate the α dependence.

The energy differences are indicated in Fig. 7.9. We concentrate on channels with $J_{123} \leq 1$ (PW = 12) and its difference to the NN+3N-full calculation (PW = 0) for $E_{\max}^{\mathrm{SRG},4} = 20/21$. The energy difference increases from 26.7 MeV for results obtained with $\alpha = 0.04$ fm^4 to 33.9 MeV for $\alpha = 0.16$ fm^4. However, the results for $\alpha = 0.16$ fm^4 have an energy difference of 23.7 MeV, which is smaller than the energy difference for $\alpha = 0.04$ fm^4. Consequently, the investigated four-body channels are not expected to remove the α dependence completely, although they might reduce it.

Similar to the previous calculations the results are far from convergence with respect to $E_{\max}^{\mathrm{SRG},4}$. While the calculations for different values of α show a similar behavior, the convergence is influenced by α. Of course, the energy difference and the effect of the induced four-body forces must vanish for $\alpha \to 0$, which makes it surprising to find the worst convergence with the smallest α. On the other hand, there is no reason for the convergence to become increasingly better or worse for higher values of α. As we have seen, the convergence with respect to $E_{\max}^{\mathrm{SRG},4}$ is not even monotonic in most of the cases.

Considering the uncertainties discussed in previous sections, these results are promising, as they show that the induced four-body forces increase the ^{16}O ground-state energy, and they might be able to reduce the α dependence. Nevertheless, we should keep in mind that these results are far from convergence with respect to $E_{\max}^{\mathrm{SRG},4}$, we omitted all channels with $J_{123} \geq 2$ and, although we expect the energy difference to be independent of $N_{\max}$, the results could still be different in a fully converged IT-NCSM calculation.

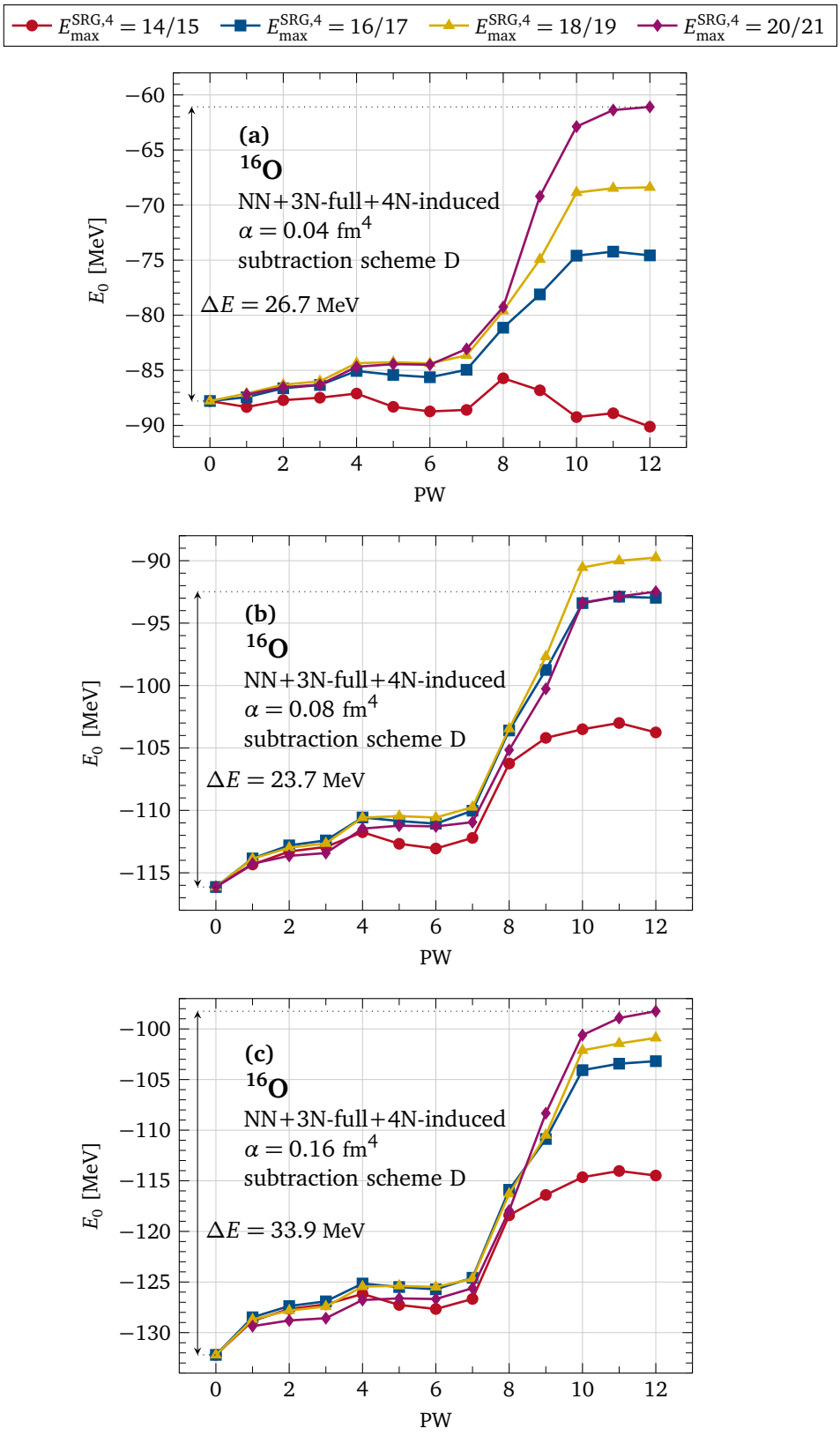


Figure 7.9: Comparison of different α values using NN+3N-full+4N-induced interactions. The ^{16}O ground-state energy is plotted over the number of included four-body channels. ΔE denotes the difference between the PW = 12 and the PW = 0 result for $E_{\max}^{\mathrm{SRG},4} = 20/21$. Furthermore, $\hbar\omega = 24$ MeV, $N_{\max} = 2$, $E_{\max}^4 = 6$ and subtraction scheme D were used.

8 Conclusion and Outlook

In this thesis the four-body forces that are induced by evolving chiral NN+3N interactions using the SRG evolution are incorporated in (IT-)NCSM calculations. We are able to include the four-body forces explicitly in the many-body calculations. This requires a transformation from Jacobi basis, which is used for the SRG evolution, to the JT-coupled scheme, which is used for (IT-)NCSM calculation. As the latter requires a huge number of four-body matrix element to express the Hamiltonian, we are forced to use a truncation in HO energy that is lower than the corresponding truncation in the Jacobi basis. For small $N_{\max}$ this is inconsequential, as the truncation is sufficient to represent all necessary interaction matrix elements.

Using the four-body forces explicitly we performed a considerable number of benchmark calculations. We discovered that channels with larger angular momentum have a stronger effect on the energy. Unfortunately, the convergence with respect to the SRG model space is slow and it degrades with an increasing number of channels, prohibiting an inclusion of channels with $J_{123} \geq 2$ for any reliable calculation. Even for calculations using all channels with $J_{123} \leq 1$ we cannot reach convergence with respect to $E_{\max}^{\mathrm{SRG},4}$. We found huge differences when varying subtraction schemes or $\hbar\omega$ values, which can be attributed to the convergence issues. A NN+3N-induced+4N-induced calculation also points out the negative effect of the two-body forces on convergence with the four-body SRG model-space size, even though they are not expected to yield a sizable four-body contribution when converged with respect to the SRG model space and all relevant four-body channels are included [14].

Using the subtraction scheme D with $\hbar\omega = 24\,\mathrm{MeV}$ we investigated the α dependence including the four-body forces for small NCSM model spaces. As NN+3N-full calculations become more and more attractive with an increasing value of α, we expected the four-body force to become more repulsive to suppress this effect. Indeed, we find the ground-state energy of ^{16}O to be higher compared to calculations without four-body forces. Overall, this effect becomes stronger for larger values of α, as expected. Although, we find the induced four-body force to be less repulsive for $\alpha = 0.08\,\mathrm{fm}^4$ than for $\alpha = 0.04\,\mathrm{fm}^4$. Comparing the total shift to the NN+3N-full calculations, it seems to be approximately of the correct size, when including all $J_{123} \leq 1$ channels. Nevertheless, a ground-state calculation cannot be completely accurate, as we cannot get a complete convergence with respect to the SRG model-space size. Furthermore, the effect of channels with larger angular momentum cannot be explored at the moment, as we cannot reach convergence with respect to the SRG model-space size for $J_{123} \geq 2$. The results, however, do look promising and indicate that the inclusion of four-body forces can mitigate the α dependence of the NN+3N-full calculations.

For testing the effects of induced four-body forces we also used an approximate approach, which reduced the induced four-body force to an effective three-body one. While the results obtained with this method are repulsive, as expected, it is an uncontrolled approximation, which, most likely, will not be pursued further, as the explicit inclusion of four-body forces gives more accurate results.

There are multiple possibilities to improve the results. The most problematic obstacle for a fully converged calculation is the SRG model-space size. Using more computational power or improving the implementation of the SRG evolution we might be able to push the current maximum for $E_{\max}^{\mathrm{SRG},4}$ to larger values. It is also possible to investigate other subtraction schemes.

Once we have four-body matrix elements that reliably yield improvements, multiple applications are possible. We already plan the implementation of a normal-ordering (NO) approximation, reducing the four-body forces to three-body or even two-body ones. The NO approximation has already been shown to yield good results in the three-body case [6] and reducing the four-body to a three- or two-body interaction allows us to use many-body methods that cannot handle explicit four-body forces yet, which are the majority of the many-body methods available. In this case, we do not require an explicit representation of the four-body force in the JT-coupled scheme, which eliminates the constraint regarding the basis truncation. We have already derived the formulae necessary for a NO approximation involving four-body forces, they are presented in appendix B.

Furthermore, the effect of four-body forces on the ground state and excited states of other nuclei can be investigated, as well as the influence on other observables. Especially in combination with a NO approximation, we could calculate observables for heavier nuclei, where we expect the induced four-body forces to have a sizable effect.

Appendix

A Antisymmetrizer Matrix Elements

In this chapter we will derive the antisymmetrization operator matrix elements in the partially antisymmetric four-body Jacobi basis. In order to do that we will first rewrite the antisymmetrizier using transposition operators, $\tau_{i,j}$, which exchange particles i and j. As the state is already antisymmetric in the first three particles, we just need to antisymmetrize it with respect to the fourth particle, yielding

$$\begin{aligned}\mathcal{A} &= \tfrac{1}{4}\left(1-\tau_{1,4}-\tau_{2,4}-\tau_{3,4}\right) && \text{(A.1)}\\ &= \tfrac{1}{4}\left(1-\tau_{1,3}\tau_{3,4}\tau_{1,3}-\tau_{2,3}\tau_{3,4}\tau_{2,3}-\tau_{3,4}\right) && \text{(A.2)}\\ &= \tfrac{1}{4}\left(1-3\tau_{3,4}\right). && \text{(A.3)}\end{aligned}$$

Here, we used the antisymmetry of the first three particles,

$$\tau_{1,3}=\tau_{2,3}=-1, \tag{A.4}$$

to simplify the expression. The calculation of the antisymmetrizer is thus reduced to the calculation of the transposition operator. We will split it into three parts,

$$\tau_{3,4}=\tau_{3,4}^{C}\tau_{3,4}^{S}\tau_{3,4}^{T}, \tag{A.5}$$

which act on coordinate ($\tau_{3,4}^{C}$), spin ($\tau_{3,4}^{S}$) and isospin space ($\tau_{3,4}^{T}$). To do that we need to separate the quantum numbers that depend on the second and third Jacobi coordinates from the remaining ones, as these are the quantum numbers that depend on the third and fourth particle. Furthermore, coordinate, spin and isospin parts need to be separated. We start by making the partial antisymmetrization explicit using the three-body CFPs:

$$\begin{aligned}&\left|E_{123}J_{123}M_{J_{123}}T_{123}M_{T_{123}}k_{123}\right\rangle && \text{(A.6)}\\ &=\sum_{k_{12}} c_{k_{12}}^{E_{12},J_{12},T_{12},i_{12}}\left|N_1N_2N_3;\left\{\left[\left(L_1S_1\right)J_1\left(L_2\tfrac{1}{2}\right)J_2\right]J_{12}\left(L_3\tfrac{1}{2}\right)J_3\right\}J_{123}M_{J_{123}}\right\rangle\left|\left[\left(T_1\tfrac{1}{2}\right)T_{12}\tfrac{1}{2}\right]T_{123}M_{T_{123}}\right\rangle. && \text{(A.7)}\end{aligned}$$

We handle the angular momentum and isospin parts of the basis separately from here on. Having separated the quantum numbers corresponding to the second and third Jacobi coordinate, we derive the matrix elements of the transposition operators.

Angular Momentum

We recouple the state to separate the quantum numbers that belong to the second and third Jacobi coordinate using a 6-J symbol, resulting in a state were J_2 and J_3 are coupled to J_{23}, while J_1 is separate.

$$\begin{aligned}&\left|\left\{\left[\left(L_1S_1\right)J_1\left(L_2\tfrac{1}{2}\right)J_2\right]J_{12}\left(L_3\tfrac{1}{2}\right)J_3\right\}J_{123}M_{J_{123}}\right\rangle && \text{(A.8)}\\ &=\sum_{J_{23}}(-1)^{J_1+J_2+J_3+J_{123}}\hat{J}_{12}\hat{J}_{23}\begin{Bmatrix}J_1 & J_2 & J_{12}\\ J_3 & J_{123} & J_{23}\end{Bmatrix}\\ &\quad\left|\left\{\left(L_1S_1\right)J_1\left[\left(L_2\tfrac{1}{2}\right)J_2\left(L_3\tfrac{1}{2}\right)J_3\right]J_{23}\right\}J_{123}M_{J_{123}}\right\rangle. && \text{(A.9)}\end{aligned}$$

We decouple J_1 and J_{23} using CGCs,

$$\begin{aligned}&=\sum_{J_{23}}\sum_{M_{J_1},M_{J_{23}}}(-1)^{J_1+J_2+J_3+J_{123}}\hat{J}_{12}\hat{J}_{23}\begin{Bmatrix}J_1 & J_2 & J_{12}\\ J_3 & J_{123} & J_{23}\end{Bmatrix}\mathrm{c}\begin{pmatrix}J_1 & J_{23} & \middle| & J_{123}\\ M_{J_1} & M_{J_{23}} & & M_{J_{123}}\end{pmatrix}\\ &\quad\left|\left(L_1S_1\right)J_1M_{J_1}\right\rangle\left|\left[\left(L_2\tfrac{1}{2}\right)J_2\left(L_3\tfrac{1}{2}\right)J_3\right]J_{23}M_{J_{23}}\right\rangle, && \text{(A.10)}\end{aligned}$$

and change the coupling scheme to LS-coupling for the quantum numbers defined with respect to the second and third Jacobi coordinates and decouple spin and orbital angular momentum:

$$
\begin{aligned}
=&\sum_{J_{23}}\sum_{M_{J_1},M_{J_{23}}}\sum_{L_{23},S_{23}}\sum_{M_{L_{23}},M_{S_{23}}}(-1)^{J_1+J_2+J_3+J_{123}}\hat{J}_{12}\hat{J}_{23}\hat{J}_2\hat{J}_3\hat{L}_{23}\hat{S}_{23}\begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ L_3 & \frac{1}{2} & J_3 \\ L_{23} & S_{23} & J_{23}\end{Bmatrix} \\
&\begin{Bmatrix} J_1 & J_2 & J_{12} \\ J_3 & J_{123} & J_{23}\end{Bmatrix}\mathrm{c}\begin{pmatrix} J_1 & J_{23} & \vert & J_{123} \\ M_{J_1} & M_{J_{23}} & \vert & M_{J_{123}}\end{pmatrix}\mathrm{c}\begin{pmatrix} L_{23} & S_{23} & \vert & J_{23} \\ M_{L_{23}} & M_{S_{23}} & \vert & M_{J_{23}}\end{pmatrix} \\
&\left|\left(L_1S_1\right)J_1M_{J_1}\right\rangle\left|\left(L_2L_3\right)L_{23}M_{L_{23}}\right\rangle\left|\left(\tfrac{1}{2}\tfrac{1}{2}\right)S_{23}M_{S_{23}}\right\rangle,
\end{aligned}
\tag{A.11}
$$

which results in the desired separation.

Isospin

Again we separate the second and third Jacobi coordinates' quantum numbers from the rest by changing the coupling scheme and decoupling of the result using a 6-J symbol and a CGC:

$$
\begin{aligned}
&\left|\left[\left(T_1\tfrac{1}{2}\right)T_{12}\tfrac{1}{2}\right]T_{123}M_{T_{123}}\right\rangle \\
&=\sum_{T_{23}}(-1)^{1+T_1+T_{123}}\hat{T}_{12}\hat{T}_{23}\begin{Bmatrix} T_1 & \frac{1}{2} & T_{12} \\ \frac{1}{2} & T_{123} & T_{23}\end{Bmatrix}\left|\left[T_1\left(\tfrac{1}{2}\tfrac{1}{2}\right)T_{23}\right]T_{123}M_{T_{123}}\right\rangle \qquad \text{(A.12)} \\
&=\sum_{T_{23}}\sum_{M_{T_1},M_{T_{23}}}(-1)^{1+T_1+T_{123}}\hat{T}_{12}\hat{T}_{23}\begin{Bmatrix} T_1 & \frac{1}{2} & T_{12} \\ \frac{1}{2} & T_{123} & T_{23}\end{Bmatrix}\mathrm{c}\begin{pmatrix} T_1 & T_{23} & \vert & T_{123} \\ M_{T_1} & M_{T_{23}} & \vert & M_{T_{123}}\end{pmatrix}\left|T_1M_{T_1}\right\rangle\left|\left(\tfrac{1}{2}\tfrac{1}{2}\right)T_{23}M_{T_{23}}\right\rangle. \qquad \text{(A.13)}
\end{aligned}
$$

We now start constructing the matrix elements for the spin, isospin and spatial part, using the separated basis parts derived above.

Spin / Isospin Matrix Elements

A general matrix element for the spin-transposition operator can be derived by decoupling both states:

$$
\begin{aligned}
&\left\langle\left(s_i's_j'\right)S_{ij}'M_{S_{ij}}'\middle|\,\tau_{i,j}^S\,\middle|\left(s_is_j\right)S_{ij}M_{S_{ij}}\right\rangle \\
&=\sum_{m_{s_i}',m_{s_j}'}\sum_{m_{s_i},m_{s_j}}\mathrm{c}\begin{pmatrix} s_i' & s_j' & \vert & S_{ij}' \\ m_{s_i}' & m_{s_j}' & \vert & M_{S_{ij}}'\end{pmatrix}\mathrm{c}\begin{pmatrix} s_i & s_j & \vert & S_{ij} \\ m_{s_i} & m_{s_j} & \vert & M_{S_{ij}}\end{pmatrix}\left\langle s_i'm_{s_i'},s_j'm_{s_j'}\middle|\,\tau_{i,j}^S\,\middle|s_im_{s_i},s_jm_{s_j}\right\rangle,
\end{aligned}
\tag{A.14}
$$

which yields δ-functions if the transposition operator ist applied to the decoupled state.

$$
\begin{aligned}
&=\sum_{m_{s_i}',m_{s_j}'}\sum_{m_{s_i},m_{s_j}}\mathrm{c}\begin{pmatrix} s_i' & s_j' & \vert & S_{ij}' \\ m_{s_i}' & m_{s_j}' & \vert & M_{S_{ij}}'\end{pmatrix}\mathrm{c}\begin{pmatrix} s_i & s_j & \vert & S_{ij} \\ m_{s_i} & m_{s_j} & \vert & M_{S_{ij}}\end{pmatrix}\delta_{s_i',s_j}\delta_{m_{s_i}',m_{s_j}}\delta_{s_j',s_i}\delta_{m_{s_j}',m_{s_i}} \qquad \text{(A.15)} \\
&=\delta_{s_i',s_j}\delta_{s_j',s_i}\sum_{m_{s_i},m_{s_j}}\mathrm{c}\begin{pmatrix} s_j & s_i & \vert & S_{ij}' \\ m_{s_j} & m_{s_i} & \vert & M_{S_{ij}}'\end{pmatrix}\mathrm{c}\begin{pmatrix} s_i & s_j & \vert & S_{ij} \\ m_{s_i} & m_{s_j} & \vert & M_{S_{ij}}\end{pmatrix}. \qquad \text{(A.16)}
\end{aligned}
$$

We can use the symmetry relation of the CGCs (Eq. 3.9) and afterwards use their orthogonality relation Eq. (3.7), which yields

$$
\begin{aligned}
&=\delta_{s_i',s_j}\delta_{s_j',s_i}(-1)^{s_i+s_j-S_{ij}}\sum_{m_{s_i},m_{s_j}}\mathrm{c}\begin{pmatrix} s_j & s_i & \vert & S_{ij}' \\ m_{s_j} & m_{s_i} & \vert & M_{S_{ij}}'\end{pmatrix}\mathrm{c}\begin{pmatrix} s_j & s_i & \vert & S_{ij} \\ m_{s_j} & m_{s_i} & \vert & M_{S_{ij}}\end{pmatrix} \qquad \text{(A.17)} \\
&=\delta_{s_i',s_j}\delta_{s_j',s_i}\delta_{S_{ij}',S_{ij}}\delta_{M_{S_{ij}}',M_{S_{ij}}}(-1)^{S_{ij}-s_i-s_j}. \qquad \text{(A.18)}
\end{aligned}
$$

The same holds true for the isospin matrix elements and therefore we end up with the following two formulae for the matrix elements of the transposition operators acting on spin and isospin:

$$\left\langle \left(\tfrac{1}{2}\tfrac{1}{2}\right) S'_{23} M'_{S_{23}} \middle| \tau^S_{34} \middle| \left(\tfrac{1}{2}\tfrac{1}{2}\right) S_{23} M_{S_{23}} \right\rangle = (-1)^{S_{23}-1} \delta_{S_{23},S'_{23}} \delta_{M_{S_{23}},M'_{S_{23}}} \tag{A.19}$$

$$\left\langle \left(\tfrac{1}{2}\tfrac{1}{2}\right) T'_{23} M'_{T_{23}} \middle| \tau^T_{34} \middle| \left(\tfrac{1}{2}\tfrac{1}{2}\right) T_{23} M_{T_{23}} \right\rangle = (-1)^{T_{23}-1} \delta_{T_{23},T'_{23}} \delta_{M_{T_{23}},M'_{T_{23}}} . \tag{A.20}$$

Keep in mind that (iso-)spin quantum numbers with indices 2 and 3 represent the third and fourth particle's (iso-)spin in Jacobi basis.

Spatial Matrix Elements

The transposition operator τ^C_{34} leads to a change in the coordinates ξ_2 and ξ_3,

$$\xi_2 = \sqrt{\tfrac{2}{3}} \left[\tfrac{1}{2} (r_1 + r_2) - r_4 \right] \tag{A.21}$$

$$\xi_3 = \sqrt{\tfrac{3}{4}} \left[\tfrac{1}{3} (r_1 + r_2 + r_4) - r_3 \right], \tag{A.22}$$

and the quantum numbers are defined with respect to these coordinates now. They can be expanded in terms of the Jacobi coordinates of the primed state (which are the standard Jacobi coordinates):

$$\xi'_2 = \sqrt{\tfrac{2}{3}} \left[\tfrac{1}{2} (r_1 + r_2) - r_3 \right] \tag{A.23}$$

$$\xi'_3 = \sqrt{\tfrac{3}{4}} \left[\tfrac{1}{3} (r_1 + r_2 + r_3) - r_4 \right]. \tag{A.24}$$

Using the matrix from Eq. (3.28) for the conversion between these coordinates, we can easily solve for $d = \frac{1}{8}$, which yields

$$\begin{pmatrix} \xi'_2 \\ \xi'_3 \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{8}{1+8}} & \sqrt{\frac{1}{1+8}} \\ \sqrt{\frac{8}{1+8}} & -\sqrt{\frac{8}{1+8}} \end{pmatrix} \begin{pmatrix} \xi_2 \\ \xi_3 \end{pmatrix} \tag{A.25}$$

for the transformation between the two sets of coordinates. The matrix element for the spatial part is simply the overlap between the two coordinate systems, which can be expressed using an HOB:

$$\left\langle N'_2 N'_3; (L'_2 L'_3) L'_{23} M'_{L_{23}} \middle| \tau^C_{34} \middle| N_2 N_3; (L_2 L_3) L_{23} M_{L_{23}} \right\rangle = \delta_{L_{23},L'_{23}} \delta_{M_{L_{23}},M'_{L_{23}}} \ll N'_2 L'_2, N'_3 L'_3 | N_2 L_2, N_3 L_3; L_{23} \gg_{\frac{1}{8}} . \tag{A.26}$$

Complete Expression

Assembling the matrix elements derived in this chapter, we obtain an expression for the complete matrix element of the transposition operator. Keep in mind that there are parts of the basis that do not involve the third or fourth particle. These parts are not affected by the transposition operator and thus yield Kronecker deltas, since our states are orthonormal.

$$\begin{aligned}
&\left\langle E'_{123} J'_{123} M'_{J_{123}} T'_{123} M'_{T_{123}} k'_{123} \middle| \tau_{34} \middle| E_{123} J_{123} M_{J_{123}} T_{123} M_{T_{123}} k_{123} \right\rangle \\
&= \sum_{k_{12}} \sum_{J_{23}} \sum_{M_{J_1}, M_{J_{23}}} \sum_{L_{23}, S_{23}} \sum_{M_{L_{23}}, M_{S_{23}}} \sum_{T_{23}} \sum_{M_{T_1}, M_{T_{23}}} \sum_{k'_{12}} \sum_{J'_{23}} \sum_{M'_{J_1}, M'_{J_{23}}} \sum_{L'_{23}, S'_{23}} \sum_{M'_{L_{23}}, M'_{S_{23}}} \sum_{T'_{23}} \sum_{M'_{T_1}, M'_{T_{23}}} c^{E_{12}, J_{12}, T_{12}, i_{12}}_{k_{12}} c^{E'_{12}, J'_{12}, T'_{12}, i'_{12}}_{k'_{12}} \\
&\quad \hat{J}_{12} \hat{J}_{23} \hat{J}_2 \hat{J}_3 \hat{L}_{23} \hat{S}_{23} \hat{T}_{12} \hat{T}_{23} \hat{J}'_{12} \hat{J}'_{23} \hat{J}'_2 \hat{J}'_3 \hat{L}'_{23} \hat{S}'_{23} \hat{T}'_{12} \hat{T}'_{23} (-1)^{J_1+J_2+J_3+J_{123}+T_1+T_{123}+J'_1+J'_2+J'_3+J'_{123}+T'_1+T'_{123}+T_{23}+S_{23}} \\
&\quad \begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ L_3 & \frac{1}{2} & J_3 \\ L_{23} & S_{23} & J_{23} \end{Bmatrix} \begin{Bmatrix} L'_2 & \frac{1}{2} & J'_2 \\ L'_3 & \frac{1}{2} & J'_3 \\ L'_{23} & S'_{23} & J_{23'} \end{Bmatrix} \begin{Bmatrix} J_1 & J_2 & J_{12} \\ J_3 & J_{123} & J_{23} \end{Bmatrix} \begin{Bmatrix} T_1 & \frac{1}{2} & T_{12} \\ \frac{1}{2} & T_{123} & T_{23} \end{Bmatrix} \begin{Bmatrix} J'_1 & J'_2 & J'_{12} \\ J'_3 & J'_{123} & J'_{23} \end{Bmatrix} \begin{Bmatrix} T'_1 & \frac{1}{2} & T'_{12} \\ \frac{1}{2} & T'_{123} & T'_{23} \end{Bmatrix} \\
&\quad \mathrm{c} \begin{pmatrix} J_1 & J_{23} & J_{123} \\ M_{J_1} & M_{J_{23}} & M_{J_{123}} \end{pmatrix} \mathrm{c} \begin{pmatrix} L_{23} & S_{23} & J_{23} \\ M_{L_{23}} & M_{S_{23}} & M_{J_{23}} \end{pmatrix} \mathrm{c} \begin{pmatrix} T_1 & T_{23} & T_{123} \\ M_{T_1} & M_{T_{23}} & M_{T_{123}} \end{pmatrix} \mathrm{c} \begin{pmatrix} J'_1 & J'_{23} & J'_{123} \\ M'_{J_1} & M'_{J_{23}} & M'_{J_{123}} \end{pmatrix} \\
&\quad \mathrm{c} \begin{pmatrix} L'_{23} & S'_{23} & J'_{23} \\ M'_{L_{23}} & M'_{S_{23}} & M'_{J_{23}} \end{pmatrix} \mathrm{c} \begin{pmatrix} T'_1 & T'_{23} & T'_{123} \\ M'_{T_1} & M'_{T_{23}} & M'_{T_{123}} \end{pmatrix} \ll N'_2 L'_2, N'_3 L'_3 | N_2 L_2, N_3 L_3; L_{23} \gg_{\frac{1}{8}} \\
&\quad \delta_{N_1,N'_1} \delta_{L_1,L'_1} \delta_{S_1,S'_1} \delta_{J_1,J'_1} \delta_{M_{J_1},M'_{J_1}} \delta_{T_1,T'_1} \delta_{M'_{T_1},M_{T_1}} \delta_{S_{23},S'_{23}} \delta_{M_{S_{23}},M'_{S_{23}}} \delta_{T_{23},T'_{23}} \delta_{M_{T_{23}},M'_{T_{23}}} \delta_{L_{23},L'_{23}} \delta_{M_{L_{23}},M'_{L_{23}}} .
\end{aligned} \tag{A.27}$$

This formula can be greatly simplified by using the δ-functions and the orthogonality relation of the CGCs (Eq. 3.7). For simplifying the factors we need to keep in mind that $2J_1$, $2T_1$, $2T_{123}$ and $2J_{123}$ are even. Note that $\delta_{E_{123},E'_{123}}$ was added to make the conservation of the relative harmonic-oscillator energy explicit. It results from the energy conservation of the HOB and from the δ-functions for N_1 and L_1:

$$
\begin{aligned}
=&\delta_{E_{123},E'_{123}}\delta_{J_{123},J'_{123}}\delta_{M_{J_{123}},M'_{J_{123}}}\delta_{T_{123},T'_{123}}\delta_{M_{T_{123}},M'_{T_{123}}}\sum_{k_{12}}\sum_{J_{23}}\sum_{L_{23},S_{23}}\sum_{T_{23}}\sum_{k'_{12}}c_{k_{12}}^{E_{12},J_{12},T_{12},i_{12}}c_{k'_{12}}^{E'_{12},J'_{12},T'_{12},i'_{12}}\\
&\hat{J}_{12}\hat{T}_{12}\hat{J}_2\hat{J}_3\hat{J}'_{12}\hat{T}'_{12}\hat{J}'_2\hat{J}'_3\hat{J}^2_{23}\hat{L}^2_{23}\hat{S}^2_{23}\hat{T}^2_{23}(-1)^{J_2+J_3+J'_2+J'_3+T_{23}+S_{23}}\\
&\begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ L_3 & \frac{1}{2} & J_3 \\ L_{23} & S_{23} & J_{23}\end{Bmatrix}\begin{Bmatrix} L'_2 & \frac{1}{2} & J'_2 \\ L'_3 & \frac{1}{2} & J'_3 \\ L_{23} & S_{23} & J_{23}\end{Bmatrix}\begin{Bmatrix} J_1 & J_2 & J_{12} \\ J_3 & J_{123} & J_{23}\end{Bmatrix}\begin{Bmatrix} T_1 & \frac{1}{2} & T_{12} \\ \frac{1}{2} & T_{123} & T_{23}\end{Bmatrix}\begin{Bmatrix} J_1 & J'_2 & J'_{12} \\ J'_3 & J_{123} & J_{23}\end{Bmatrix}\begin{Bmatrix} T_1 & \frac{1}{2} & T'_{12} \\ \frac{1}{2} & T_{123} & T_{23}\end{Bmatrix}\\
&\ll N'_2L'_2,N'_3L'_3|N_2L_2,N_3L_3;L_{23}\gg_{\frac{1}{8}}\delta_{N_1,N'_1}\delta_{L_1,L'_1}\delta_{S_1,S'_1}\delta_{J_1,J'_1}\delta_{T_1,T'_1}.
\end{aligned}
\tag{A.28}
$$

We can carry out the sum over T_{23} using Eq. (3.23). Furthermore we reorder the formula to separate it into two parts:

$$
\begin{aligned}
&= \delta_{E_{123},E'_{123}}\delta_{J_{123},J'_{123}}\delta_{M_{J_{123}},M'_{J_{123}}}\delta_{T_{123},T'_{123}}\delta_{M_{T_{123}},M'_{T_{123}}}\sum_{k_{12}}\sum_{L_{23}}\sum_{k'_{12}}c_{k_{12}}^{E_{12},J_{12},T_{12},i_{12}}c_{k'_{12}}^{E'_{12},J'_{12},T'_{12},i'_{12}}\\
&\hat{J}_{12}\hat{T}_{12}\hat{J}_2\hat{J}_3\hat{J}'_{12}\hat{T}'_{12}\hat{J}'_2\hat{J}'_3\hat{L}^2_{23}(-1)^{T_{12}+T'_{12}}\begin{Bmatrix}\frac{1}{2} & T_{123} & T_{12}\\ \frac{1}{2} & T_1 & T'_{12}\end{Bmatrix}\ll N'_2L'_2,N'_3L'_3|N_2L_2,N_3L_3;L_{23}\gg_{\frac{1}{8}}\delta_{N_1,N'_1}\delta_{L_1,L'_1}\delta_{S_1,S'_1}\delta_{J_1,J'_1}\delta_{T_1,T'_1}\Bigg\}\text{(I)}\\
&\sum_{J_{23}}\sum_{S_{23}}\hat{J}^2_{23}\hat{S}^2_{23}(-1)^{J_2+J_3+J'_2+J'_3+S_{23}}\begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ L_3 & \frac{1}{2} & J_3 \\ L_{23} & S_{23} & J_{23}\end{Bmatrix}\begin{Bmatrix} L'_2 & \frac{1}{2} & J'_2 \\ L'_3 & \frac{1}{2} & J'_3 \\ L_{23} & S_{23} & J_{23}\end{Bmatrix}\begin{Bmatrix} J_1 & J_2 & J_{12} \\ J_3 & J_{123} & J_{23}\end{Bmatrix}\begin{Bmatrix} J_1 & J'_2 & J'_{12} \\ J'_3 & J_{123} & J_{23}\end{Bmatrix}\Bigg\}\text{(II)}
\end{aligned}
\tag{A.29}
$$

We will simplify part (II) now, starting by reordering rows and columns of the 9-J symbols.

$$
\text{(II)} = \sum_{J_{23}}\sum_{S_{23}}\hat{J}^2_{23}\hat{S}^2_{23}(-1)^{1+L_2+L_3+J'_2+J'_3+L_{23}+J_{23}}\begin{Bmatrix} L_2 & J_2 & \frac{1}{2} \\ L_3 & J_3 & \frac{1}{2} \\ L_{23} & J_{23} & S_{23}\end{Bmatrix}\begin{Bmatrix} L'_3 & J'_3 & \frac{1}{2} \\ L'_2 & J'_2 & \frac{1}{2} \\ L_{23} & J_{23} & S_{23}\end{Bmatrix}\begin{Bmatrix} J_1 & J_2 & J_{12} \\ J_3 & J_{123} & J_{23}\end{Bmatrix}\begin{Bmatrix} J_1 & J'_2 & J'_{12} \\ J'_3 & J_{123} & J_{23}\end{Bmatrix}.
\tag{A.30}
$$

Using Eq. (3.24) we can carry out the sum over S_{23}

$$
= \sum_{J_{23}}\sum_{P}\hat{J}^2_{23}\hat{P}^2(-1)^{L_2+L'_2+J'_2+J'_2}\begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ L_{23} & L'_3 & L'_2 \\ L_3 & J'_3 & P\end{Bmatrix}\begin{Bmatrix} J_3 & J_{23} & J_2 \\ \frac{1}{2} & J'_2 & L'_2 \\ L_3 & J'_3 & P\end{Bmatrix}\begin{Bmatrix} J_1 & J_2 & J_{12} \\ J_3 & J_{123} & J_{23}\end{Bmatrix}\begin{Bmatrix} J_1 & J'_2 & J'_{12} \\ J'_3 & J_{123} & J_{23}\end{Bmatrix}.
\tag{A.31}
$$

We expand the second 9-J symbol using Eq. (3.21) after we reorder its columns. Note that $2K$ is an even number and therefore the phase factor from Eq. (3.21) vanishes.

$$
\begin{aligned}
&= \sum_{J_{23}}\sum_{P}\sum_{K}\hat{J}^2_{23}\hat{P}^2\hat{K}^2(-1)^{L_2+L'_2+J'_2+J'_2}\begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ L_{23} & L'_3 & L'_2 \\ L_3 & J'_3 & P\end{Bmatrix}\begin{Bmatrix} J_2 & L'_2 & P \\ L_3 & J'_3 & K\end{Bmatrix}\begin{Bmatrix} J_3 & \frac{1}{2} & L_3 \\ L'_2 & K & J'_2\end{Bmatrix}\begin{Bmatrix} J_{23} & J'_2 & J'_3 \\ K & J_2 & J_3\end{Bmatrix}\\
&\begin{Bmatrix} J_1 & J_2 & J_{12} \\ J_3 & J_{123} & J_{23}\end{Bmatrix}\begin{Bmatrix} J_1 & J'_2 & J'_{12} \\ J'_3 & J_{123} & J_{23}\end{Bmatrix}.
\end{aligned}
\tag{A.32}
$$

We use Eq. (3.21) again to carry out the sum over J_{23}. This time it is used to create a new 9-J symbol instead of expanding it:

$$
= \sum_{P}\sum_{K}\hat{P}^2\hat{K}^2(-1)^{L_2+L'_2+J'_2+J'_2}\begin{Bmatrix} L_2 & \frac{1}{2} & J_2 \\ L_{23} & L'_3 & L'_2 \\ L_3 & J'_3 & P\end{Bmatrix}\begin{Bmatrix} J_1 & J_2 & J_{12} \\ J'_2 & K & J_3 \\ J'_{12} & J'_3 & J_{123}\end{Bmatrix}\begin{Bmatrix} J_2 & L'_2 & P \\ L_3 & J'_3 & K\end{Bmatrix}\begin{Bmatrix} J_3 & \frac{1}{2} & L_3 \\ L'_2 & K & J'_2\end{Bmatrix}.
\tag{A.33}
$$

After reordering the rows in the first 9-J symbol we use Eq. (3.25) to carry out the sum over P.

$$= \sum_K \hat{K}^2 (-1)^{L_2+L_2'+J_2'+J_2'} \begin{Bmatrix} J_1 & J_2 & J_{12} \\ J_2' & K & J_3 \\ J_{12}' & J_3' & J_{123} \end{Bmatrix} \begin{Bmatrix} J_3 & \frac{1}{2} & L_3 \\ L_2' & K & J_2' \end{Bmatrix} \begin{Bmatrix} L_3 & L_2' & K \\ L_3' & L_2 & L_{23} \end{Bmatrix} \begin{Bmatrix} L_3' & L_2 & K \\ J_2 & J_3' & \frac{1}{2} \end{Bmatrix}. \tag{A.34}$$

Including part (I) again, we get the following final result for a matrix element of the transposition operator:

$$\begin{aligned} &\left\langle E_{123}' J_{123}' M_{J_{123}}' T_{123}' M_{T_{123}}' k_{123}' \right| \tau_{34} \left| E_{123} J_{123} M_{J_{123}} T_{123} M_{T_{123}} k_{123} \right\rangle \\ &= \delta_{E_{123},E_{123}'} \delta_{J_{123},J_{123}'} \delta_{M_{J_{123}},M_{J_{123}}'} \delta_{T_{123},T_{123}'} \delta_{M_{T_{123}},M_{T_{123}}'} \sum_{k_{12}} \sum_{L_{23}} \sum_{k_{12}'} \sum_K c_{k_{12}}^{E_{12},J_{12},T_{12},i_{12}} c_{k_{12}'}^{E_{12}',J_{12}',T_{12}',i_{12}'} \\ &\quad \hat{J}_{12} \hat{T}_{12} \hat{J}_2 \hat{J}_3 \hat{J}_{12}' \hat{T}_{12}' \hat{J}_2' \hat{J}_3' \hat{L}_{23}^2 \hat{K}^2 (-1)^{T_{12}+T_{12}'+L_2+L_2'+J_2'+J_2'} \\ &\quad \begin{Bmatrix} J_1 & J_2 & J_{12} \\ J_2' & K & J_3 \\ J_{12}' & J_3' & J_{123} \end{Bmatrix} \begin{Bmatrix} J_3 & \frac{1}{2} & L_3 \\ L_2' & K & J_2' \end{Bmatrix} \begin{Bmatrix} L_3 & L_2' & K \\ L_3' & L_2 & L_{23} \end{Bmatrix} \begin{Bmatrix} L_3' & L_2 & K \\ J_2 & J_3' & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & T_{123} & T_{12} \\ \frac{1}{2} & T_1 & T_{12}' \end{Bmatrix} \\ &\quad \ll N_2' L_2', N_3' L_3' | N_2 L_2, N_3 L_3; L_{23} \gg_{\frac{1}{8}} \delta_{N_1,N_1'} \delta_{L_1,L_1'} \delta_{S_1,S_1'} \delta_{J_1,J_1'} \delta_{T_1,T_1'}. \end{aligned} \tag{A.35}$$

This formula has already been derived by Navrátil and Barrett [37]. When comparing their formula to ours it is important to keep in mind that their definition of the HOB is different from the one we used.

B Normal Ordering

The normal ordering approximation allows us to reduce four-body interactions to zero-, one-, two- and three-body ones. This allows for an inclusion of states with higher total HO energy in many-body calculations. More importantly, many-body methods that cannot handle four-body forces explicitly become accessible. However, it is an approximation that can significantly influence the results. As of today, we have no results using this scheme, nevertheless the derivation of the relevant formulae is given in this chapter.

For discussing normal ordering, the following notation, which differs from the rest of this work, is advantegeous. We will work with matrix elements of single-particle states using the following abbreviation:

$$V_{qsuw}^{prtv} = {}_a\langle prtv \left| V_{4\mathrm{N}} \right| qsuw \rangle_a . \tag{B.1}$$

Furthermore we use creation and annihilation operators to express interactions,

$$V_{4\mathrm{N}} = \frac{1}{4!^2} \sum_{\substack{prtv \\ qsuw}} V_{qsuw}^{prtv} A_{qsuw}^{prtv}, \tag{B.2}$$

where we used the following abbreviation for particle number conserving operators:

$$A_{qsuw}^{prtv} = a_p^\dagger a_r^\dagger a_t^\dagger a_v^\dagger a_w a_u a_s a_q. \tag{B.3}$$

In general, a normal ordering procedure changes a string of creation and annihilation operators into a specific order. This normal order is defined by a reference state. If this state is the vacuum, all creation operators should be on the left of all annihilation operators. However, if we have a reference state $|\Phi\rangle$, which is constructed from a set of occupied states, we need to define quasi-particle creation and annihilation operators.

Using the reference state, we define the quasi-particle annihilation operators as those operators that annihilate the state:

$$\tilde{a}_p |\Phi\rangle = 0, \tag{B.4}$$

which defines the following relation between normal and quasi-particle operatores:

$$a_p^\dagger = \begin{cases} \tilde{a}_p & \text{if } p \text{ is occupied} \\ \tilde{a}_p^\dagger & \text{otherwise} \end{cases} \qquad a_p = \begin{cases} \tilde{a}_p^\dagger & \text{if } p \text{ is occupied} \\ \tilde{a}_p & \text{otherwise} \end{cases} \tag{B.5}$$

where $\tilde{a}_p^\dagger$ and $\tilde{a}_p$ denote the quasi-particle creation and annihilation operators, respectively. We can now define a string of operators to be in normal order with respect to $|\Phi\rangle$, if all quasi-particle creation operators are on the left of all quasi-particle annihilation operators. A string of normal ordered quasi-particle operators is abbreviated by:

$$\tilde{A}_{qsuw}^{prtv} = (-1)^P \tilde{a}_p^\dagger \tilde{a}_r^\dagger \tilde{a}_t^\dagger \tilde{a}_v^\dagger \tilde{a}_w \tilde{a}_u \tilde{a}_s \tilde{a}_q, \tag{B.6}$$

where P denotes the number of permutations that is needed to change the operator order from vacuum normal order to quasi-particle normal order.

Using Wick's theorem we can express a string of operators that is in vacuum normal order by strings of operators that are in normal order with respect to the reference state. This ultimately yields the following expression [38]:

$$A_{qsuw}^{prtv} = \gamma_{qsuw}^{prtv} + \mathbb{A}(\gamma_{qsu}^{prt} \tilde{A}_w^v) + \mathbb{A}(\gamma_{qs}^{pr} \tilde{A}_{uw}^{tv}) + \mathbb{A}(\gamma_q^p \tilde{A}_{suw}^{rtv}) + \tilde{A}_{qsuw}^{prtv}, \tag{B.7}$$

where γ denotes a density matrix, which can be defined in the following way:

$$\gamma_{qs\ldots}^{pr\ldots} = \langle \Phi | A_{qs\ldots}^{pr\ldots} | \Phi \rangle . \tag{B.8}$$

A detailed derivation of Eq. (B.7) has been done by Gebrerufael, see pp. 20 - 26 of Ref. [15]. If the reference state is a Slater-determinant of single-particle states, density-matrices can be evaluated easily:

$$\gamma_q^p = \langle \Phi | A_q^p | \Phi \rangle = o_p \delta_{p,q}, \tag{B.9}$$

$$\gamma_{qs}^{pr} = \langle \Phi | A_{qs}^{pr} | \Phi \rangle = o_p o_r (\delta_{p,q}\delta_{r,s} - \delta_{p,s}\delta_{r,s}), \tag{B.10}$$

$$\gamma_{qsu}^{prt} = \langle \Phi | A_{qsu}^{prt} | \Phi \rangle = o_p o_r o_t (\delta_{p,q}\delta_{r,s}\delta_{t,u} + \delta_{p,u}\delta_{r,q}\delta_{t,s} + \delta_{p,s}\delta_{r,u}\delta_{t,q} - \delta_{p,q}\delta_{r,u}\delta_{t,s} - \delta_{p,s}\delta_{r,q}\delta_{t,u} - \delta_{p,u}\delta_{r,s}\delta_{t,q}), \tag{B.11}$$

where we used occupation numbers o_x given by:

$$o_x = \begin{cases} 1 & \text{if } x \text{ is occupied} \\ 0 & \text{otherwise} \end{cases} \tag{B.12}$$

The fourth density-matrix was omitted for brevity.

Note that the index antisymmetrization operator, $\mathbb{A}$, is defined differently from the usual antysimmetrizer. It sums over all different permutations of upper and lower indices, introducing a minus sign for odd permutations. As γ and $\tilde{A}$ are antisymmetric in their upper/lower indices, exchanging their indices does not contribute to the sum. Furthermore, it does not exchange upper and lower indices and no additional factors are introduced. A more detailed description is given by Gebrerufael [15]. Using this definition, we can calculate the number of terms $\mathbb{A}$ will produce:

$$\begin{aligned} \mathbb{A}(\gamma^{prt}_{qsu}\tilde{A}^{v}_{w}) &: \binom{4}{1}^2 = 4^2, \\ \mathbb{A}(\gamma^{pr}_{qs}\tilde{A}^{tv}_{uw}) &: \binom{4}{2}^2 = 6^2, \\ \mathbb{A}(\gamma^{p}_{q}\tilde{A}^{rtv}_{suw}) &: \binom{4}{3}^2 = 4^2. \end{aligned}$$

Note that all three expressions are antisymmetric in p,r,t and v, as well as in q,s,u and w.

Inserting Eq. (B.7) in Eq. (B.2) yields the following expression for the four-body force:

$$V_{4N} = \frac{1}{4!^2} \sum_{\substack{prtv \\ qsuw}} V^{prtv}_{qsuw} A^{prtv}_{qsuw} \tag{B.13}$$

$$= \frac{1}{4!^2} \sum_{\substack{prtv \\ qsuw}} V^{prtv}_{qsuw} \gamma^{prtv}_{qsuw} + \frac{4^2}{4!^2} \sum_{\substack{prtv \\ qsuw}} V^{prtv}_{qsuw} \gamma^{prt}_{qsu} \tilde{A}^{v}_{w} + \frac{6^2}{4!^2} \sum_{\substack{prtv \\ qsuw}} V^{prtv}_{qsuw} \gamma^{pr}_{qs} \tilde{A}^{tv}_{uw} + \frac{4^2}{4!^2} \sum_{\substack{prtv \\ qsuw}} V^{prtv}_{qsuw} \gamma^{p}_{q} \tilde{A}^{rtv}_{suw} + \frac{1}{4!^2} \sum_{\substack{prtv \\ qsuw}} V^{prtv}_{qsuw} \tilde{A}^{prtv}_{qsuw}, \tag{B.14}$$

where we used the fact that V is antisymmetric in its upper and lower indices. Used together with the antisymmetry of $\mathbb{A}$, it is easy to see that all the terms that are produced by $\mathbb{A}$ yield the same expression, as we can always reorder the indices of V accordingly and then rename the sum's indices. This expression is usually written as:

$$V_{4N} = W + \sum_{\substack{v \\ w}} W^{v}_{w} \tilde{A}^{v}_{w} + \frac{1}{2!^2} \sum_{\substack{tv \\ uw}} W^{tv}_{uw} \tilde{A}^{tv}_{uw} + \frac{1}{3!^2} \sum_{\substack{rtv \\ suw}} W^{rtv}_{suw} \tilde{A}^{rtv}_{suw} + \frac{1}{4!^2} \sum_{\substack{prtv \\ qsuw}} W^{prtv}_{qsuw} \tilde{A}^{prtv}_{qsuw} \tag{B.15}$$

with:

$$\begin{aligned} W &= \frac{1}{4!^2} \sum_{\substack{prtv \\ qsuw}} V^{prtv}_{qsuw} \gamma^{prtv}_{qsuw} & W^{v}_{w} &= \frac{1}{3!^2} \sum_{\substack{prt \\ qsu}} V^{prtv}_{qsuw} \gamma^{prt}_{qsu} \\ W^{tv}_{uw} &= \frac{1}{2!^2} \sum_{\substack{pr \\ qs}} V^{prtv}_{qsuw} \gamma^{pr}_{qs} & W^{rtv}_{suw} &= \sum_{\substack{p \\ q}} V^{prtv}_{qsuw} \gamma^{p}_{q} \\ W^{prtv}_{qsuw} &= V^{prtv}_{qsuw} \end{aligned}$$

If we use a Slater-determinant of single-particle states as the reference state, this can be simplified by inserting Eqs. (B.9) to (B.12). The normal ordered matrix elements thus read:

$$\begin{aligned} W &= \frac{1}{4!} \sum_{prtv} V^{prtv}_{prtv} o_p o_r o_t o_v & W^{v}_{w} &= \frac{1}{3!} \sum_{prt} V^{prtv}_{prtw} o_p o_r o_t \\ W^{tv}_{uw} &= \frac{1}{2!} \sum_{pr} V^{prtv}_{pruw} o_p o_r & W^{rtv}_{suw} &= \sum_{p} V^{prtv}_{psuw} o_p \\ W^{prtv}_{qsuw} &= V^{prtv}_{qsuw}, \end{aligned}$$

where we used the antisymmetry of V to sum over all contributions.

This transformation can be inverted, by normal ordering the constructed interaction, which is normal ordered with respect to $|\Phi\rangle$, with respect to the vacuum again, which yields:

$$\frac{1}{4!^2}\sum_{\substack{prtv\\qsuw}} W^{prtv}_{qsuw}\tilde{A}^{prtv}_{qsuw} = {}^4U + \sum_{\substack{v\\w}} {}^4U^v_w A^v_w + \frac{1}{2!^2}\sum_{\substack{tv\\uw}} {}^4U^{tv}_{uw}A^{tv}_{uw} + \frac{1}{3!^2}\sum_{\substack{rtv\\suw}} {}^4U^{rtv}_{suw}A^{rtv}_{suw} + \frac{1}{4!^2}\sum_{\substack{prtv\\qsuw}} {}^4U^{prtv}_{qsuw}A^{prtv}_{qsuw} \tag{B.16}$$

$$\frac{1}{3!^2}\sum_{\substack{rtv\\suw}} W^{rtv}_{suw}\tilde{A}^{rtv}_{suw} = {}^3U + \sum_{\substack{v\\w}} {}^3U^v_w A^v_w + \frac{1}{2!^2}\sum_{\substack{tv\\uw}} {}^3U^{tv}_{uw}A^{tv}_{uw} + \frac{1}{3!^2}\sum_{\substack{rtv\\suw}} {}^3U^{rtv}_{suw}A^{rtv}_{suw} \tag{B.17}$$

$$\frac{1}{2!^2}\sum_{\substack{tv\\uw}} W^{tv}_{uw}\tilde{A}^{tv}_{uw} = {}^2U + \sum_{\substack{v\\w}} {}^2U^v_w A^v_w + \frac{1}{2!^2}\sum_{\substack{tv\\uw}} {}^2U^{tv}_{uw}A^{tv}_{uw} \tag{B.18}$$

$$\sum_{\substack{v\\w}} W^v_w\tilde{A}^v_w = {}^1U + \sum_{\substack{v\\w}} {}^1U^v_w A^v_w \tag{B.19}$$

$$W = {}^0U \tag{B.20}$$

with

$${}^4U = \frac{1}{4!^2}\sum_{\substack{prtv\\qsuw}} W^{prtv}_{qsuw}\tilde{\gamma}^{prtv}_{qsuw} \qquad {}^4U^v_w = \frac{1}{3!^2}\sum_{\substack{prt\\qsu}} W^{prtv}_{qsuw}\tilde{\gamma}^{prt}_{qsu} \qquad {}^4U^{tv}_{uw} = \frac{1}{2!^2}\sum_{\substack{pr\\qs}} W^{prtv}_{qsuw}\tilde{\gamma}^{pr}_{qs} \qquad {}^4U^{rtv}_{suw} = \sum_{\substack{p\\q}} W^{prtv}_{qsuw}\tilde{\gamma}^{p}_{q} \qquad {}^4U^{prtv}_{qsuw} = W^{prtv}_{qsuw}$$

$${}^3U = \frac{1}{3!^2}\sum_{\substack{rtv\\suw}} W^{rtv}_{suw}\tilde{\gamma}^{rtv}_{suw} \qquad {}^3U^v_w = \frac{1}{2!^2}\sum_{\substack{rt\\su}} W^{rtv}_{suw}\tilde{\gamma}^{rt}_{su} \qquad {}^3U^{tv}_{uw} = \sum_{\substack{r\\s}} W^{rtv}_{suw}\tilde{\gamma}^{r}_{s} \qquad {}^3U^{rtv}_{suw} = W^{rtv}_{suw}$$

$${}^2U = \frac{1}{2!^2}\sum_{\substack{tv\\uw}} W^{tv}_{uw}\tilde{\gamma}^{tv}_{uw} \qquad {}^2U^v_w = \sum_{\substack{t\\u}} W^{tv}_{uw}\tilde{\gamma}^{t}_{u} \qquad {}^2U^{tv}_{uw} = W^{tv}_{uw}$$

$${}^1U = \sum_{\substack{v\\w}} W^v_w\tilde{\gamma}^v_w \qquad {}^1U^v_w = W^v_w$$

$${}^0U = W$$

The $\tilde{\gamma}$ differ from the previous case. This time the operators are ordered with respect to $|\Phi\rangle$ and we normal order with respect to the vacuum.

$$\begin{aligned}
\tilde{\gamma}^p_q &= \langle 0|\tilde{A}^p_q|0\rangle = -\gamma^p_q \\
\tilde{\gamma}^{pr}_{qs} &= \langle 0|\tilde{A}^{pr}_{qs}|0\rangle = \gamma^{pr}_{qs} \\
\tilde{\gamma}^{prt}_{qsu} &= \langle 0|\tilde{A}^{prt}_{qsu}|0\rangle = -\gamma^{prt}_{qsu} \\
\tilde{\gamma}^{prtv}_{qsuw} &= \langle 0|\tilde{A}^{prtv}_{qsuw}|0\rangle = \gamma^{prtv}_{qsuw}
\end{aligned}$$

We can get this result by putting a minus sign in front of every δ-function. The minus signs originate from the definition of the string of quasi-particle operators (Eq. B.6). If we now add up the different contributions we will get the original four-body interaction:

$${}^0U + {}^1U + {}^2U + {}^3U + {}^4U = 0 \tag{B.21}$$

$${}^1U^v_w + {}^2U^v_w + {}^3U^v_w + {}^4U^v_w = 0 \tag{B.22}$$

$${}^2U^{tv}_{uw} + {}^3U^{tv}_{uw} + {}^4U^{tv}_{uw} = 0 \tag{B.23}$$

$${}^3U^{rtv}_{suw} + {}^4U^{rtv}_{suw} = 0 \tag{B.24}$$

$${}^4U^{prtv}_{qsuw} = V^{prtv}_{qsuw} \tag{B.25}$$

At this point we can apply the approximation. If the reference state is a good description of the target state, we expect the four-body matrix elements, W^{prtv}_{qsuw}, to be small. We therefore simply omit the four-body part and then normal order the interaction with respect to the vacuum again, which yields an effective three-body force:

$$
\begin{aligned}
{}^{\text{eff}}V &= {}^0U + {}^1U + {}^2U + {}^3U = -{}^4U &&= -\frac{1}{4!}\sum_{prtv} V^{prtv}_{prtv}\, o_p o_r o_t o_v && \text{(B.26)}\\
{}^{\text{eff}}V^v_w &= {}^1U^v_w + {}^2U^v_w + {}^3U^v_w &&= -{}^4U^v_w = \frac{1}{3!}\sum_{prt} V^{prtv}_{prtw}\, o_p o_r o_t && \text{(B.27)}\\
{}^{\text{eff}}V^{tv}_{uw} &= {}^2U^{tv}_{uw} + {}^3U^{tv}_{uw} &&= -{}^4U^{tv}_{uw} = -\frac{1}{2!}\sum_{pr} V^{prtv}_{pruw}\, o_p o_r && \text{(B.28)}\\
{}^{\text{eff}}V^{rtv}_{suw} &= {}^3U^{rtv}_{suw} &&= -{}^4U^{rtv}_{suw} = \sum_{p} V^{prtv}_{psuw}\, o_p && \text{(B.29)}\\
{}^{\text{eff}}V^{prtv}_{qsuw} &= 0 && && \text{(B.30)}\\
\Rightarrow\quad {}^{\text{eff}}V_{4N} &= {}^{\text{eff}}V + \sum_{\substack{v\\w}} {}^{\text{eff}}V^v_w A^v_w + \frac{1}{2!^2}\sum_{\substack{tv\\uw}} {}^{\text{eff}}V^{tv}_{uw} A^{tv}_{uw} + \frac{1}{3!^2}\sum_{\substack{rtv\\suw}} {}^{\text{eff}}V^{rtv}_{suw} A^{rtv}_{suw} && && \text{(B.31)}
\end{aligned}
$$

B.1 JT-Coupled Scheme

As our matrix elements are stored in the JT-coupled scheme (see Sec. 4.2), we will derive different versions of Eqs. (B.26) to (B.29), using coupled matrix elements. The single-particle states are assumed to be HO states, e.g., the state p has quantum numbers n_p,l_p,j_p,m_{j_p} and m_{t_p}. During the derivation we will separate the angular momentum projection quantum number. The remaining quantum numbers, n_p,l_p,j_p and m_{t_p}, are abbreviated by $\tilde{p}$. Furthermore the occupation number is written as $o_{\tilde{p}}$, if it is independent of m_{j_p}. Note that the coupled four-body matrix elements are diagonal in J and T. Additionally, they are completely independent of M_J and M_T. In the following sections we will use the standard notation for matrix elements again. Keep in mind that the abbreviation α_{prtv} does not include any projection quantum numbers.

Zero-Body Operator

The zero-body part is simply a sum over all possible m-scheme states and we can use CGCs to change the expression to the JT-coupled scheme.

$$
\begin{aligned}
\langle 0|{}^{\text{eff}}V|0\rangle &= -\frac{1}{4!}\sum_{prtv}\left\langle prtv\right|V\left|prtv\right\rangle o_p o_r o_t o_v\\
&= -\frac{1}{4!}\sum_{prtv}\sum_{J_{pr},T_{pr}}\sum_{J_{prt},T_{prt}}\sum_{J'_{pr},T'_{pr}}\sum_{J'_{prt},T'_{prt}}\sum_{J,T}\sum_{M_{J_{pr}},M_{T_{pr}}}\sum_{M_{J_{prt}},M_{T_{prt}}}\sum_{M_J,M_T}\\
&\quad \mathrm{c}\begin{pmatrix} j_p & j_r & J_{pr}\\ m_{j_p} & m_{j_r} & M_{J_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} j_p & j_r & J'_{pr}\\ m_{j_p} & m_{j_r} & M_{J_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{pr} & j_t & J_{prt}\\ M_{J_{pr}} & m_{j_t} & M_{J_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J'_{pr} & j_t & J'_{prt}\\ M_{J_{pr}} & m_{j_t} & M_{J_{prt}}\end{pmatrix}\\
&\quad \mathrm{c}\begin{pmatrix} J_{prt} & j_v & J\\ M_{J_{prt}} & m_{j_v} & M_J\end{pmatrix}\mathrm{c}\begin{pmatrix} J'_{prt} & j_v & J\\ M_{J_{prt}} & m_{j_v} & M_J\end{pmatrix}\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & T_{pr}\\ m_{t_p} & m_{t_r} & M_{T_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & T'_{pr}\\ m_{t_p} & m_{t_r} & M_{T_{pr}}\end{pmatrix}\\
&\quad \mathrm{c}\begin{pmatrix} T_{pr} & \frac{1}{2} & T_{prt}\\ M_{T_{pr}} & m_{t_t} & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{pr} & \frac{1}{2} & T'_{prt}\\ M_{T_{pr}} & m_{t_t} & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} & T\\ M_{T_{prt}} & m_{t_v} & M_T\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{prt} & \frac{1}{2} & T\\ M_{T_{prt}} & m_{t_v} & M_T\end{pmatrix}\\
&\quad {}_a\left\langle E'JM_JTM_T\alpha'_{prtv}\right|V\left|EJM_JTM_T\alpha_{prtv}\right\rangle_a o_p o_r o_t o_v. \qquad \text{(B.32)}
\end{aligned}
$$

We now concentrate on closed-shell nuclei, which means that $o_p ... o_v$ are independent of angular momentum projection quantum numbers. We can therefore split the sum in the following way: $\sum_p \rightarrow \sum_{\tilde{p},m_{j_p}}$, where $\tilde{p}$ denotes the remaining quantum numbers.

$$
\begin{aligned}
=&-\frac{1}{4!}\sum_{\tilde{p}\tilde{r}\tilde{t}\tilde{v}}\sum_{m_{j_p}}\sum_{m_{j_r}}\sum_{m_{j_t}}\sum_{m_{j_v}}\sum_{J_{pr},T_{pr}}\sum_{J_{prt},T_{prt}}\sum_{J'_{pr},T'_{pr}}\sum_{J'_{prt},T'_{prt}}\sum_{J,T}\sum_{M_{J_{pr}},M_{T_{pr}}}\sum_{M_{J_{prt}},M_{T_{prt}}}\sum_{M_J,M_T}\\
&\mathrm{c}\begin{pmatrix} j_p & j_r & | & J_{pr} \\ m_{j_p} & m_{j_r} & | & M_{J_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} j_p & j_r & | & J'_{pr} \\ m_{j_p} & m_{j_r} & | & M_{J_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{pr} & j_t & | & J_{prt} \\ M_{J_{pr}} & m_{j_t} & | & M_{J_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J'_{pr} & j_t & | & J'_{prt} \\ M_{J_{pr}} & m_{j_t} & | & M_{J_{prt}}\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} J_{prt} & j_v & | & J \\ M_{J_{prt}} & m_{j_v} & | & M_J\end{pmatrix}\mathrm{c}\begin{pmatrix} J'_{prt} & j_v & | & J \\ M_{J_{prt}} & m_{j_v} & | & M_J\end{pmatrix}\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & | & T_{pr} \\ m_{t_p} & m_{t_r} & | & M_{T_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & | & T'_{pr} \\ m_{t_p} & m_{t_r} & | & M_{T_{pr}}\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} T_{pr} & \frac{1}{2} & | & T_{prt} \\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{pr} & \frac{1}{2} & | & T'_{prt} \\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} & | & T \\ M_{T_{prt}} & m_{t_v} & | & M_T\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{prt} & \frac{1}{2} & | & T \\ M_{T_{prt}} & m_{t_v} & | & M_T\end{pmatrix}\\
&{}_a\left\langle E'JM_JTM_T\alpha'_{prtv}\right| V \left|EJM_JTM_T\alpha_{prtv}\right\rangle_a o_{\tilde{p}}o_{\tilde{r}}o_{\tilde{t}}o_{\tilde{v}}.
\end{aligned}
\tag{B.33}
$$

We can now use the orthogonality relation of the Clebsch-Gordan coefficients (Eq. 3.7) to carry out the sums over the single-particle angular momentum projection quantum numbers.

$$
\begin{aligned}
=&-\frac{1}{4!}\sum_{\tilde{p}\tilde{r}\tilde{t}\tilde{v}}\sum_{J_{pr},T_{pr}}\sum_{J_{prt},T_{prt}}\sum_{T'_{pr}}\sum_{T'_{prt}}\sum_{J,T}\sum_{M_{T_{pr}}}\sum_{M_{T_{prt}}}\sum_{M_T}(2J+1)\\
&\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & | & T_{pr} \\ m_{t_p} & m_{t_r} & | & M_{T_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & | & T'_{pr} \\ m_{t_p} & m_{t_r} & | & M_{T_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{pr} & \frac{1}{2} & | & T_{prt} \\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{pr} & \frac{1}{2} & | & T'_{prt} \\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} & | & T \\ M_{T_{prt}} & m_{t_v} & | & M_T\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{prt} & \frac{1}{2} & | & T \\ M_{T_{prt}} & m_{t_v} & | & M_T\end{pmatrix}{}_a\left\langle E'JM_JTM_T\alpha'_{prtv}\right| V \left|EJM_JTM_T\alpha_{prtv}\right\rangle_a o_{\tilde{p}}o_{\tilde{r}}o_{\tilde{t}}o_{\tilde{v}}.
\end{aligned}
\tag{B.34}
$$

One-Body Operator

The approach for the one-body operator is similar, as simple coupling of the four-body m-scheme basis states yields JT-coupled scheme expressions.

$$
\langle v|^{\mathrm{eff}} V |w\rangle = \frac{1}{3!}\sum_{prt}\left\langle prtv\right| V \left|prtw\right\rangle o_p o_r o_t \tag{B.35}
$$

$$
\begin{aligned}
=&\frac{1}{3!}\sum_{prt}\sum_{J_{pr},T_{pr}}\sum_{J_{prt},T_{prt}}\sum_{J'_{pr},T'_{pr}}\sum_{J'_{prt},T'_{prt}}\sum_{J,T}\sum_{M_{J_{pr}},M_{T_{pr}}}\sum_{M_{J_{prt}},M_{T_{prt}}}\sum_{M_J,M_T}\\
&\mathrm{c}\begin{pmatrix} j_p & j_r & | & J_{pr} \\ m_{j_p} & m_{j_r} & | & M_{J_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} j_p & j_r & | & J'_{pr} \\ m_{j_p} & m_{j_r} & | & M_{J_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{pr} & j_t & | & J_{prt} \\ M_{J_{pr}} & m_{j_t} & | & M_{J_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J'_{pr} & j_t & | & J'_{prt} \\ M_{J_{pr}} & m_{j_t} & | & M_{J_{prt}}\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} J_{prt} & j_v & | & J \\ M_{J_{prt}} & m_{j_v} & | & M_J\end{pmatrix}\mathrm{c}\begin{pmatrix} J'_{prt} & j_w & | & J \\ M_{J_{prt}} & m_{j_w} & | & M_J\end{pmatrix}\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & | & T_{pr} \\ m_{t_p} & m_{t_r} & | & M_{T_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & | & T'_{pr} \\ m_{t_p} & m_{t_r} & | & M_{T_{pr}}\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} T_{pr} & \frac{1}{2} & | & T_{prt} \\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{pr} & \frac{1}{2} & | & T'_{prt} \\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} & | & T \\ M_{T_{prt}} & m_{t_v} & | & M_T\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{prt} & \frac{1}{2} & | & T \\ M_{T_{prt}} & m_{t_w} & | & M_T\end{pmatrix}\\
&{}_a\left\langle E'JM_JTM_T\alpha_{prtv}\right| V \left|EJM_JTM_T\alpha_{prtw}\right\rangle_a o_p o_r o_t.
\end{aligned}
\tag{B.36}
$$

We can easily see that $m_{j_v} = m_{j_w}$ and $m_{t_v} = m_{t_w}$. Furthermore, we split the sum, which is only allowed for closed-shell nuclei:

$$
\begin{aligned}
=&\frac{1}{3!}\sum_{\tilde{p}\tilde{r}\tilde{t}}\sum_{m_{j_p}}\sum_{m_{j_r}}\sum_{m_{j_t}}\sum_{J_{pr},T_{pr}}\sum_{J_{prt},T_{prt}}\sum_{J'_{pr},T'_{pr}}\sum_{J'_{prt},T'_{prt}}\sum_{J,T}\sum_{M_{J_{pr}},M_{T_{pr}}}\sum_{M_{J_{prt}},M_{T_{prt}}}\sum_{M_J,M_T}\delta_{m_{j_v},m_{j_w}}\delta_{m_{t_v},m_{t_w}}\\
&\mathrm{c}\begin{pmatrix} j_p & j_r & | & J_{pr}\\ m_{j_p} & m_{j_r} & | & M_{J_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} j_p & j_r & | & J'_{pr}\\ m_{j_p} & m_{j_r} & | & M_{J_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{pr} & j_t & | & J_{prt}\\ M_{J_{pr}} & m_{j_t} & | & M_{J_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J'_{pr} & j_t & | & J'_{prt}\\ M_{J_{pr}} & m_{j_t} & | & M_{J_{prt}}\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} J_{prt} & j_v & | & J\\ M_{J_{prt}} & m_{j_v} & | & M_J\end{pmatrix}\mathrm{c}\begin{pmatrix} J'_{prt} & j_w & | & J\\ M_{J_{prt}} & m_{j_v} & | & M_J\end{pmatrix}\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & | & T_{pr}\\ m_{t_p} & m_{t_r} & | & M_{T_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & | & T'_{pr}\\ m_{t_p} & m_{t_r} & | & M_{T_{pr}}\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} T_{pr} & \frac{1}{2} & | & T_{prt}\\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{pr} & \frac{1}{2} & | & T'_{prt}\\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} & | & T\\ M_{T_{prt}} & m_{t_v} & | & M_T\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{prt} & \frac{1}{2} & | & T\\ M_{T_{prt}} & m_{t_v} & | & M_T\end{pmatrix}\\
&{}_a\left\langle E'JM_JTM_T\alpha_{prtv}\right| V\left|EJM_JTM_T\alpha_{prtw}\right\rangle_a o_{\tilde{p}}o_{\tilde{r}}o_{\tilde{t}}.
\end{aligned}
\tag{B.37}
$$

Using symmetry relations for the Clebsch-Gordan coefficients (Eqs. 3.9, 3.10) and using their orthogonality relation (Eq. 3.7), we end up with:

$$
\begin{aligned}
=&\frac{1}{3!}\sum_{\tilde{p}\tilde{r}\tilde{t}}\sum_{J_{pr},T_{pr}}\sum_{J_{prt},T_{prt}}\sum_{J'_{pr},T'_{pr}}\sum_{J'_{prt},T'_{prt}}\sum_{J,T}\sum_{M_{T_{pr}}}\sum_{M_{T_{prt}}}\sum_{M_T}\delta_{j_v,j_w}\delta_{m_{j_v},m_{j_w}}\delta_{m_{t_v},m_{t_w}}\frac{2J+1}{2j_v+1}\\
&\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & | & T_{pr}\\ m_{t_p} & m_{t_r} & | & M_{T_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & | & T'_{pr}\\ m_{t_p} & m_{t_r} & | & M_{T_{pr}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{pr} & \frac{1}{2} & | & T_{prt}\\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{pr} & \frac{1}{2} & | & T'_{prt}\\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} & | & T\\ M_{T_{prt}} & m_{t_v} & | & M_T\end{pmatrix}\mathrm{c}\begin{pmatrix} T'_{prt} & \frac{1}{2} & | & T\\ M_{T_{prt}} & m_{t_v} & | & M_T\end{pmatrix}{}_a\left\langle E'JM_JTM_T\alpha_{prtv}\right| V\left|EJM_JTM_T\alpha_{prtw}\right\rangle_a o_{\tilde{p}}o_{\tilde{r}}o_{\tilde{t}}.
\end{aligned}
\tag{B.38}
$$

Two-Body Operator

In the two-body case we want the resulting matrix elements to be expressed in the JT-coupled scheme as well, we therefore sum over a mixed four-body state, where the first two states are coupled to a total angular momentum and total isospin, while the last two states are separate. Using CGCs we can express the state using the four-body JT-coupled scheme:

$$
\begin{aligned}
&{}_a\left\langle n_pn_r;\left[\left(l_p\tfrac{1}{2}\right)j_p\left(l_r\tfrac{1}{2}\right)j_r\right]J_{pr}M_{J_{pr}};\left(\tfrac{1}{2}\tfrac{1}{2}\right)T_{pr}M_{T_{pr}}\right|{}^{\mathrm{eff}}V\left|n_qn_s;\left[\left(l_q\tfrac{1}{2}\right)j_q\left(l_s\tfrac{1}{2}\right)j_s\right]J_{qs}M_{J_{qs}};\left(\tfrac{1}{2}\tfrac{1}{2}\right)T_{qs}M_{T_{qs}}\right\rangle_a\\
&=-\frac{1}{2!}\sum_{tv}{}_a\left\{\left\langle n_pn_r;\left[\left(l_p\tfrac{1}{2}\right)j_p\left(l_r\tfrac{1}{2}\right)j_r\right]J_{pr}M_{J_{pr}};\left(\tfrac{1}{2}\tfrac{1}{2}\right)T_{pr}M_{T_{pr}}\right|\left\langle tv\right|\right\}\\
&\qquad{}^{\mathrm{eff}}V\left\{\left|n_qn_s;\left[\left(l_q\tfrac{1}{2}\right)j_q\left(l_s\tfrac{1}{2}\right)j_s\right]J_{qs}M_{J_{qs}};\left(\tfrac{1}{2}\tfrac{1}{2}\right)T_{qs}M_{T_{qs}}\right\rangle\left|tv\right\rangle\right\}_a o_to_v
\end{aligned}
\tag{B.39}
$$

$$
\begin{aligned}
=&-\frac{1}{2!}\sum_{tv}\sum_{J_{prt},T_{prt}}\sum_{J,T}\sum_{J_{qst},T_{qst}}\sum_{M_{J_{prt}},M_{T_{prt}}}\sum_{M_J,M_T}\sum_{M_{J_{qst}},M_{T_{qst}}}\\
&\mathrm{c}\begin{pmatrix} J_{pr} & j_t & | & J_{prt}\\ M_{J_{pr}} & m_{j_t} & | & M_{J_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{qs} & j_t & | & J_{qst}\\ M_{J_{qs}} & m_{j_t} & | & M_{J_{qst}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{prt} & j_v & | & J\\ M_{J_{prt}} & m_{j_v} & | & M_J\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{qst} & j_v & | & J\\ M_{J_{qst}} & m_{j_v} & | & M_J\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} T_{pr} & \frac{1}{2} & | & T_{prt}\\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{qs} & \frac{1}{2} & | & T_{qst}\\ M_{T_{qs}} & m_{t_t} & | & M_{T_{qst}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} & | & T\\ M_{T_{prt}} & m_{t_v} & | & M_T\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{qst} & \frac{1}{2} & | & T\\ M_{T_{qst}} & m_{t_v} & | & M_T\end{pmatrix}\\
&{}_a\left\langle E'JM_JTM_T\alpha_{prtv}\right| V\left|EJM_JTM_T\alpha_{qstv}\right\rangle_a o_to_v.
\end{aligned}
\tag{B.40}
$$

We split the sum, assuming a closed-shell nucleus and use that $M_{J_{prt}} = M_{J_{qst}}$, $M_{T_{prt}} = M_{T_{qst}}$, $M_{J_{pr}} = M_{J_{qs}}$ and $M_{T_{pr}} = M_{T_{qs}}$.

$$
\begin{aligned}
=&-\frac{1}{2!}\sum_{\tilde{t}\tilde{v}}\sum_{m_{j_t}}\sum_{m_{j_v}}\sum_{J_{prt},T_{prt}}\sum_{J,T}\sum_{J_{qst},T_{qst}}\sum_{J',T'}\sum_{M_{J_{prt}},M_{T_{prt}}}\sum_{M_J,M_T}\delta_{M_{J_{pr}},M_{J_{qs}}}\delta_{M_{T_{pr}},M_{T_{qs}}}\\
&\mathrm{c}\begin{pmatrix} J_{pr} & j_t & | & J_{prt}\\ M_{J_{pr}} & m_{j_t} & | & M_{J_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{qs} & j_t & | & J_{qst}\\ M_{J_{pr}} & m_{j_t} & | & M_{J_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{prt} & j_v & | & J\\ M_{J_{prt}} & m_{j_v} & | & M_J\end{pmatrix}\mathrm{c}\begin{pmatrix} J_{qst} & j_v & | & J\\ M_{J_{prt}} & m_{j_v} & | & M_J\end{pmatrix}\\
&\mathrm{c}\begin{pmatrix} T_{pr} & \frac{1}{2} & | & T_{prt}\\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{qs} & \frac{1}{2} & | & T_{qst}\\ M_{T_{pr}} & m_{t_t} & | & M_{T_{prt}}\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} & | & T\\ M_{T_{prt}} & m_{t_v} & | & M_T\end{pmatrix}\mathrm{c}\begin{pmatrix} T_{qst} & \frac{1}{2} & | & T\\ M_{T_{qst}} & m_{t_v} & | & M_T\end{pmatrix}\\
&{}_a\left\langle E'JM_JTM_T\alpha_{prtv}\right| V\left|EJM_JTM_T\alpha_{qstv}\right\rangle_a o_to_v.
\end{aligned}
\tag{B.41}
$$

Summing over M_J and m_{j_v} yields:

$$
\begin{aligned}
&= -\frac{1}{2!}\sum_{\tilde{t}\,\tilde{v}}\sum_{m_{j_t}}\sum_{J_{prt},T_{prt}}\sum_{J,T}\sum_{J_{qst},T_{qst}}\sum_{J',T'}\sum_{M_{J_{prt}},M_{T_{prt}}}\sum_{M_T}\delta_{M_{J_{pr}},M_{J_{qs}}}\delta_{M_{T_{pr}},M_{T_{qs}}}\delta_{J_{prt},J_{qst}}\frac{2J+1}{2J_{prt}+1}\\
&\quad \mathrm{c}\begin{pmatrix} J_{pr} & j_t \\ M_{J_{pr}} & m_{j_t}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} J_{prt} \\ M_{J_{prt}}\end{matrix}\mathrm{c}\begin{pmatrix} J_{qs} & j_t \\ M_{J_{pr}} & m_{j_t}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} J_{qst} \\ M_{J_{prt}}\end{matrix}\mathrm{c}\begin{pmatrix} T_{pr} & \frac{1}{2} \\ M_{T_{pr}} & m_{t_t}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T_{prt} \\ M_{T_{prt}}\end{matrix}\mathrm{c}\begin{pmatrix} T_{qs} & \frac{1}{2} \\ M_{T_{pr}} & m_{t_t}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T_{qst} \\ M_{T_{prt}}\end{matrix}\\
&\quad \mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} \\ M_{T_{prt}} & m_{t_v}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T \\ M_T\end{matrix}\mathrm{c}\begin{pmatrix} T_{qst} & \frac{1}{2} \\ M_{T_{prt}} & m_{t_v}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T \\ M_T\end{matrix}\\
&\quad {}_a\Big\langle E'JM_JTM_T\alpha_{prtv}\Big|\,V\,\Big|EJM_JTM_T\alpha_{qstv}\Big\rangle_a\, o_t o_v,
\end{aligned}
\tag{B.42}
$$

where we used Eq. (3.10) to reorder the quantum numbers of the CGCs before using the orthogonality relation of the CGCs. After evaluating the sums over $M_{J_{prt}}$ and m_{j_t}, again using the symmetry relation of the CGCs, we end up with:

$$
\begin{aligned}
&= -\frac{1}{2!}\sum_{\tilde{t}\,\tilde{v}}\sum_{J_{prt},T_{prt}}\sum_{J,T}\sum_{J_{qst},T_{qst}}\sum_{J',T'}\sum_{M_{T_{prt}}}\sum_{M_T}\delta_{M_{J_{pr}},M_{J_{qs}}}\delta_{M_{T_{pr}},M_{T_{qs}}}\delta_{J_{prt},J_{qst}}\delta_{J_{pr},J_{qs}}\frac{2J+1}{2J_{pr}+1}\\
&\quad \mathrm{c}\begin{pmatrix} T_{pr} & \frac{1}{2} \\ M_{T_{pr}} & m_{t_t}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T_{prt} \\ M_{T_{prt}}\end{matrix}\mathrm{c}\begin{pmatrix} T_{qs} & \frac{1}{2} \\ M_{T_{pr}} & m_{t_t}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T_{qst} \\ M_{T_{prt}}\end{matrix}\mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} \\ M_{T_{prt}} & m_{t_v}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T \\ M_T\end{matrix}\mathrm{c}\begin{pmatrix} T_{qst} & \frac{1}{2} \\ M_{T_{prt}} & m_{t_v}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T \\ M_T\end{matrix}\\
&\quad {}_a\Big\langle E'JM_JTM_T\alpha_{prtv}\Big|\,V\,\Big|EJM_JTM_T\alpha_{qstv}\Big\rangle_a\, o_t o_v.
\end{aligned}
\tag{B.43}
$$

Three-Body Operator

Here we start with the three-body state that is coupled:

$$
\begin{aligned}
&{}_a\Big\langle n_p n_r n_t;\Big\{\Big[\Big(l_p\tfrac{1}{2}\Big)j_p\Big(l_r\tfrac{1}{2}\Big)j_r\Big]J_{pr}\Big(l_t\tfrac{1}{2}\Big)j_t\Big\}J_{prt}M_{J_{prt}};\Big[\Big(\tfrac{1}{2}\tfrac{1}{2}\Big)T_{pr}\tfrac{1}{2}\Big]T_{prt}M_{T_{prt}}\Big|\\
&\qquad {}^{\mathrm{eff}}V\,\Big|n_q n_s n_u;\Big\{\Big[\Big(l_q\tfrac{1}{2}\Big)j_q\Big(l_s\tfrac{1}{2}\Big)j_s\Big]J_{qs}\Big(l_u\tfrac{1}{2}\Big)j_u\Big\}J_{qsu}M_{J_{qsu}};\Big[\Big(\tfrac{1}{2}\tfrac{1}{2}\Big)T_{qs}\tfrac{1}{2}\Big]T_{qsu}M_{T_{qsu}}\Big\rangle_a\\
&=\sum_v {}_a\Big\{\Big\langle n_p n_r n_t;\Big\{\Big[\Big(l_p\tfrac{1}{2}\Big)j_p\Big(l_r\tfrac{1}{2}\Big)j_r\Big]J_{pr}\Big(l_t\tfrac{1}{2}\Big)j_t\Big\}J_{prt}M_{J_{prt}};\Big[\Big(\tfrac{1}{2}\tfrac{1}{2}\Big)T_{pr}\tfrac{1}{2}\Big]T_{prt}M_{T_{prt}}\Big|\Big\langle v\Big|\Big\}\\
&\qquad {}^{\mathrm{eff}}V\Big\{\Big|n_q n_s n_u;\Big\{\Big[\Big(l_q\tfrac{1}{2}\Big)j_q\Big(l_s\tfrac{1}{2}\Big)j_s\Big]J_{qs}\Big(l_u\tfrac{1}{2}\Big)j_u\Big\}J_{qsu}M_{J_{qsu}};\Big[\Big(\tfrac{1}{2}\tfrac{1}{2}\Big)T_{qs}\tfrac{1}{2}\Big]T_{qsu}M_{T_{qsu}}\Big\rangle\Big|v\Big\rangle\Big\}_a\, o_v.
\end{aligned}
\tag{B.44}
$$

We separate the sum over v and couple the state:

$$
\begin{aligned}
&=\sum_{\tilde{v}}\sum_{m_{j_v}}\sum_{J,T}\sum_{M_J,M_T}\\
&\quad \mathrm{c}\begin{pmatrix} J_{prt} & j_v \\ M_{J_{prt}} & m_{j_v}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} J \\ M_J\end{matrix}\mathrm{c}\begin{pmatrix} J_{qsu} & j_v \\ M_{J_{qsu}} & m_{j_v}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} J \\ M_J\end{matrix}\mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} \\ M_{T_{prt}} & m_{t_v}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T \\ M_T\end{matrix}\mathrm{c}\begin{pmatrix} T_{qsu} & \frac{1}{2} \\ M_{T_{qsu}} & m_{t_v}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T \\ M_T\end{matrix}\\
&\quad {}_a\Big\langle E'JM_JTM_T\alpha_{prtv}\Big|\,V\,\Big|EJM_JTM_T\alpha_{qsuv}\Big\rangle_a\, o_{\tilde{v}}.
\end{aligned}
\tag{B.45}
$$

Summing over M_J and m_{j_v} yields the result:

$$
\begin{aligned}
&=\sum_{\tilde{v}}\sum_{J,T}\sum_{M_T}\delta_{J_{prt},J_{qsu}}\delta_{M_{J_{prt}},M_{J_{qsu}}}\delta_{M_{T_{prt}},M_{T_{qsu}}}\frac{2J+1}{2J_{prt}+1}\\
&\quad \mathrm{c}\begin{pmatrix} T_{prt} & \frac{1}{2} \\ M_{T_{prt}} & m_{t_v}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T \\ M_T\end{matrix}\mathrm{c}\begin{pmatrix} T_{qsu} & \frac{1}{2} \\ M_{T_{qsu}} & m_{t_v}\end{pmatrix}\begin{matrix}\\ \\ \end{matrix}\Bigg|\begin{matrix} T \\ M_T\end{matrix}\;{}_a\Big\langle E'JM_JTM_T\alpha_{prtv}\Big|\,V\,\Big|EJM_JTM_T\alpha_{qsuv}\Big\rangle_a\, o_{\tilde{v}}.
\end{aligned}
\tag{B.46}
$$

All of the derived expressions can be further simplified, if the nucleus has an even number of protons and neutrons. If that is not the case, additional approximations are necessary to get two- and three-body forces that are diagonal in isospin and independent of the isospin projection quantum number.

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