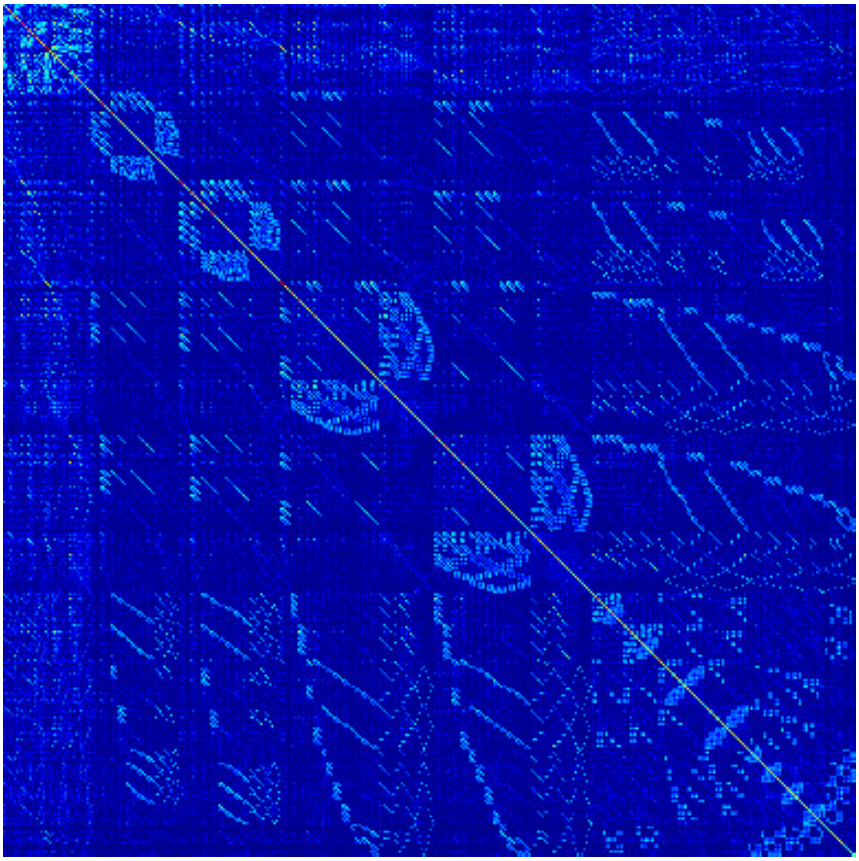

Three-Body Forces in Configuration-Interaction Methods for Nuclear Physics

Master's thesis in Physics and Astronomy

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CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden 2016

Master's thesis 2016

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Title image: Graphical representation of the full Hamiltonian matrix for ^{3}H with $N_{\max} = 4$. The Hamiltonian includes two- and three-body interactions derived from χ-EFT at NNLO [1].

Typeset in LaTeX
Gothenburg, Sweden 2016

Abstract

In this thesis, three-body forces are studied and implemented in a quantum many-body configuration-interaction method. The general importance of three-body forces in physics is discussed, providing some classical examples, before focusing in particular on their appearance in modern nuclear physics. The theoretical formalism that is needed for the implementation of three-body forces in quantum many-body systems is presented, with the angular-momentum coupling of two- and three-body systems of identical particles as main focus point. The resulting software, that is written in C, is then utilized to compute the ground-state energy of the tritium (^{3}H) and helion (^{3}He) nuclei in finite model spaces ($N_{max} \leq 8$). Results are compared with other simulations and the difference is within an acceptable tolerance. A few suggestions for future optimization of the code, such as the utilization of hash maps, are discussed.

Acknowledgements

There are several people that have been of great help throughout the work of my Masters thesis. I would very much like to thank my supervisors Christian Forssén and Andreas Ekström, who has helped and guided me with a steady hand. I would also like to give many thanks to Håkan Johansson who has been a great help with computer matters and other technical matters. I would also like to thank Dag Fahlin Strömberg, a fellow master student, who has shared office space with me throughout this project. I thank my parents, without whom I do not exist, for the support they have given despite the distance to their residence.

Tor Djärv, Gothenburg, August 2016

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1
Introduction

In this thesis, three-body forces are implemented in a quantum many-body, configuration-interaction (CI) method. The resulting software, written in C, solves the many-body Schrödinger equation to compute the ground-state energy of the tritium (^{3}H) and helion (^{3}He) nuclei with realistic nuclear interactions.
Three-body forces have a long history in physics. One of the earliest examples is the three-body problem in celestial mechanics. Gravity is inherently a two-body force, but when an extended object, such as a planet, is treated as a point-particle gravitational tidal-forces result in effective three-body forces [2]. A similar example from electrostatics is presented in section 2.1, from which the conclusion is that the reduction of degrees of freedom is the source of three- and many-body forces.
Similar to the classical case, three-body forces arise in quantum mechanics when neglecting internal degrees of freedom. A particularly relevant example is the two-pion exchange (TPE) interaction between nucleons, first studied by Fujita and Miyazawa in 1957 [3]. The Feynman diagram in figure 1.1 shows the TPE process in which one nucleon turns into a delta particle while it exchanges one pion with a neighboring nucleon. The delta particle then decays back to a nucleon while sending out a second pion that is absorbed by a third nucleon. Effectively this kind of process, with an intermediate particle excitation, involves three nucleons in the initial and final states. In an effective theory where nucleons and pions are the only fundamental constituents, three-nucleon interactions, such as the Fujita-Miyazawa term, will be present.

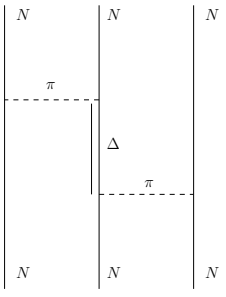

Figure 1.1: The Feynman diagram for the two-pion exchange three-nucleon interaction. The solid lines are nucleons, the double line is an intermediate delta particle, and the dashed lines are pion propagators.

The examples of three-body forces mentioned above have been results of some underlying two-body force and the removal of internal dynamics. However, there also exist fundamental three-body forces. In quantum chromodynamics, there exists a

three-gluon vertex, see figure 1.2, which can result in a three-body force between three quarks [2]. One can argue if this is a fundamental three-body force, or if it arises from a deeper physical description that we do not yet know.

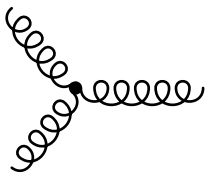

Figure 1.2: The three-gluon vertex present in quantum chromodynamics.

The implementation of three-body forces in a quantum-mechanical, many-body framework is not trivial, as will be shown in this thesis. The specific aim of this work is to solve the N-body Schrödinger equation [4]

$$\left(\sum_{i=1}^{N}\left(-\hbar^2\frac{\vec{\nabla}_i^2}{2m_i}+V_{n,i}\right)+\sum_{i<j=1}^{N}V_{nn,ij}+\sum_{i<j<k=1}^{N}V_{nnn,ijk}\right)\psi_(\vec{r}_1,\ldots,\vec{r}_N) = E\psi(\vec{r}_1,\ldots,\vec{r}_N), \tag{1.1}$$

where $V_{n,i}$, $V_{nn,i}$, and $V_{nnn,ijk}$ are the one-, two-, and thee-body forces, respectively. To achieve this goal I will employ the configuration-interaction method. See section 2.2 for more details.
In the CI method, the Hamiltonian of the many-body system is projected on a truncated many-body basis, resulting in a finite matrix representation. The Hamiltonian matrix is then diagonalized, which yields an approximation of the energy eigenvalues and the eigenstates. The software that is developed throughout this project focuses mainly on the computation of three-body force matrix elements in an angular-momentum decoupled m-scheme basis as needed for the configuration-interaction method. The starting point is a file with matrix elements in a more compact angular-momentum coupled basis. The underlying theoretical formalism is presented in chapter 3, while the software implementation is discussed in chapter 4. Results are presented in chapter 5, where I will focus on the computation of ground-state energies in ^{3}H and ^{3}He nuclei.

2

Three-Body forces in physics

In this chapter I discuss the nature and origin of three-body forces. Section 2.1 contains an example of three-body forces in classical electromagnetism. Section 2.2 deals with the origin of three-body forces in nuclear physics.

2.1 Three-body forces in classical physics

To understand what three-body forces are, I compare them to the more familiar two-body forces. A well-known example of a two-body force is Newtonian gravity. The gravitational force acting on a particle with mass m_1 at position $\vec{r}_1$ from a particle with mass m_2 located at position $\vec{r}_2$ is

$$\vec{F}(\vec{r}_1, \vec{r}_2) = G\frac{m_1 m_2(\vec{r}_2 - \vec{r}_1)}{|\vec{r}_1 - \vec{r}_2|^3}, \tag{2.1}$$

where G is the gravitational constant that determines the strength of the force. The force $\vec{F}$ is a function of the positions $\vec{r}_1$ and $\vec{r}_2$, and incidentally their masses.
There are no forces in classical physics that are intrinsically of three-body character. However, neglecting the internal dynamics of a composite object can induce effective three-body forces. To illustrate this, I have constructed an example from electrostatics.
Consider a system of two electrical charges, each with charge q, placed at $\vec{r}_1$ and $\vec{r}_2$, and an electrical dipole with dipole moment $\vec{p}$, free to rotate, at a position $\vec{r}$. This is illustrated in figure 2.1. The external electric field $\vec{E}$ on the dipole from the two charges is

$$\vec{E} = \frac{q}{4\pi\epsilon_0}\left(\frac{\vec{r} - \vec{r}_1}{|\vec{r} - \vec{r}_1|^3} + \frac{\vec{r} - \vec{r}_2}{|\vec{r} - \vec{r}_2|^3}\right) \tag{2.2}$$

Since we assume the static case, the torque on the dipole $\vec{\tau} = \vec{p} \times \vec{E}$ must vanish. This implies that the dipole moment must be parallel with the external electric field hence we have $\vec{p} = p\frac{\vec{E}}{|\vec{E}|}$.
The potential energy of the dipole in the electric field is

$$V = \vec{p}\vec{E} = p|\vec{E}| = \frac{qp}{4\pi\epsilon_0}\sqrt{\left(\frac{1}{|\vec{r}_1 - \vec{r}|^4} + \frac{1}{|\vec{r}_2 - \vec{r}|^4} + 2\frac{(\vec{r} - \vec{r}_1)\cdot(\vec{r} - \vec{r}_2)}{|\vec{r} - \vec{r}_1|^3|\vec{r} - \vec{r}_2|^3}\right)}. \tag{2.3}$$

Since a force is $\vec{F} = -\nabla V$, we can see that this V is a non-trivial function that depends on the dipole's position and the two charges positions and is therefore what we earlier defined as a three-body force, or in this case three-body potential.

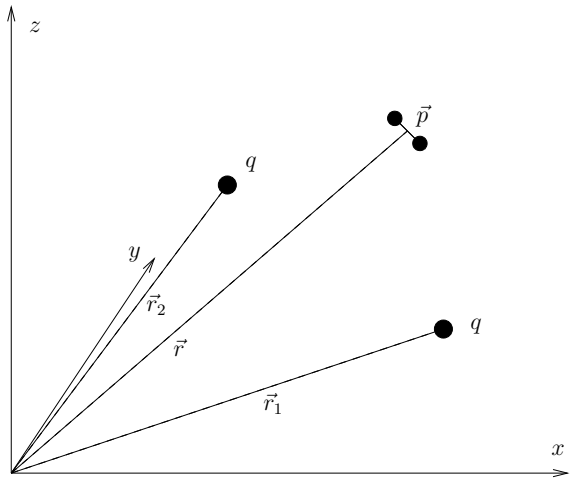

Figure 2.1: The arrangement with two electrical charges and one electric dipole.

This examples demonstrates that three-body forces arise when the internal degrees of freedom of an object is neglected. In this case the orientation of the dipole.

2.2 Three-body forces in nuclear physics

So far three-body forces have been discussed in the light of classical physics, however the atomic nucleus must be studied within the framework of quantum mechanics. The time-independent Schrödinger equation [4] is given by

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle\,, \tag{2.4}$$

where $\hat{H}$ is the Hamiltonian and ψ is the wave function.
A system of N interacting particles, with the canonical coordinates $\vec{r}_i$ and momentum $\vec{p}_i$ for $i = 1, \ldots, N$, can be described with the Hamiltonian

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m_i} + V(\vec{r}_1, \ldots, \vec{r}_N), \tag{2.5}$$

where m_i is the mass of particle i and $V(\vec{r}_1, \ldots, \vec{r}_N)$ represents the potential of the inter-particle interactions. For simplicity we now assume that the potential only depends on the positions of the particles. In the general case it will also depend on other quantum numbers. If we only include up to three-body forces, the Hamiltonian can be written on the form

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m_i} + \sum_{i=1}^{N} V_n(\vec{r}_i) + \sum_{i<j=1}^{N} V_{nn}(\vec{r}_i, \vec{r}_j) + \sum_{i<j<k=1}^{N} V_{nnn}(\vec{r}_i, \vec{r}_j, \vec{r}_k), \tag{2.6}$$

where V_n,V_{nn}, and V_{nnn} denotes the one-, two-, and three-body forces, respectively. In the quantum description the three-body force becomes a potential operator depending on three particles, in this case the position operators. From this the Schrödinger equation (2.4) becomes

$$\left(\sum_{i=1}^{N}\left(-\hbar^2\frac{\vec{\nabla}_i^2}{2m_i}+V_n(\vec{r}_i)\right)+\right.$$
$$\left.+\sum_{i<j=1}^{N}V_{nn}(\vec{r}_i,\vec{r}_j)+\sum_{i<j<k=1}^{N}V_{nnn}(\vec{r}_i,\vec{r}_j,\vec{r}_k)\right)\psi(\vec{r}_1,\ldots,\vec{r}_N)=E\psi(\vec{r}_1,\ldots,\vec{r}_N), \tag{2.7}$$

where $\vec{\nabla}_i$ is the gradient on respect of $\vec{r}_i$ and $\psi_n(\vec{r}_1,\ldots,\vec{r}_N)$ are the wave functions in coordinate space.

3

The three-body force matrix elements

The main goal of this project is to solve the Schrödinger equation for the three-nucleon systems ^{3}H and ^{3}He with the inclusion of three-nucleon forces.
In this calculation the many-body quantum states are built up by Slater determinants [5] of single-particle states, so called m-scheme states, discussed in more detail in section 3.1. The action of the Hamiltonian upon the quantum states is represented by forming a matrix between the m-scheme states. The Schrödinger equation is then solved by diagonalizing the Hamiltonian matrix.
The forces used in this project are provided in an angular-momentum coupled basis. The transformation to m-scheme is discussed in sections 3.1 and 3.2.
The behavior of three-body forces in a system with more than three particles is discussed in section 3.3. Even though this is not relevant for the current implementation of the software, it will be of importance for a future continuation of this project.
In section 3.4 I discuss the evaluation of two-body operators in a three-body basis.
In section 3.5 I describe the so-called Lawson term to treat the spurious center of mass motion of a nucleus described in single-particle coordinates.

3.1 The Many-Body Matrix Elements

The Hilbert space of A nucleons is spanned by antisymmetrized Slater determinants of single-nucleon states constructed from the harmonic-oscillator eigen basis with frequency ω. See appendix A.1 for details. The single-particle quantum numbers are n, l, s, j, m,t and t_z, where n and l are the harmonic oscillator principal quantum numbers such that $N = 2n+l$ and the Harmonic oscilator energy is $E_{nl} = \hbar\omega(N+\frac{3}{2})$, s is the spin which for the most part is omitted since $s = 1/2$ for both protons and neutrons, $|l - s| \leq j \leq l + s$ is the total angular momentum with corresponding magnetic quantum number m, t is the isospin, which is also for the most part omitted since $t = 1/2$ for both protons and neutrons, t_z is the isospin projection on the z-axis, and $t_z = -1/2$ for protons and $t_z = 1/2$ for neutrons.
A single particle state will be denoted as $|\alpha\rangle = |n, l, s, j, t, t_z, m\rangle$, and the total spin-coupled wave function is given by

$$\langle\vec{x}|\alpha\rangle = \Phi_\alpha(\vec{x}) = \sum_{m'=-l}^{l} \sum_{s_z=-\frac{1}{2}}^{\frac{1}{2}} \left(\begin{smallmatrix} l \\ m' \end{smallmatrix}, \begin{smallmatrix} 1/2 \\ s_z \end{smallmatrix} \middle| \begin{smallmatrix} j \\ m \end{smallmatrix}\right) \psi_{nlm'}(\vec{x})\chi_{s_z}\xi_{t_z} \tag{3.1}$$

where $\psi_{nlm'}(\vec{x})$ is the harmonic oscillator wave function, χ_{s_z} is the spin wave function and ξ_{t_z} is the isospin wave function. The angular-momentum coupling is described by the Clebsch-Gordan coefficients. Observe that since different nucleons may have different masses the t_z quantum number may affect $\psi_{nlm}(\vec{x})$ as well.

3.1.1 The m-scheme representation

Two different bases can be employed to span the many-nucleon Hilbert space: 1) a basis with coupled angular momentum or 2) the so-called m-scheme basis with uncoupled angular momentum. In the isospin formalism all nucleons are seen as one species of fermions, which requires that all the basis states are antisymmetric in exchange of any two particles.
Consider the m-scheme basis for a system with A nucleons. Assume that we are working in the isospin formalism. If no antisymmetrization is enforced then the basis states could be written as tensor products of single particles states,

$$|\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_A) = |\alpha_1\rangle_1 \otimes |\alpha_2\rangle_2 \otimes \cdots \otimes |\alpha_A\rangle_A \tag{3.2}$$

where α_k are single particle states, as described earlier, while the subscripted number outside the ket indicates which particle. When enforcing antisymmetrization, we have to make sure that $P_{i,j}|\Phi\rangle = -|\Phi\rangle$ where $P_{i,j}$ is an operator that exchanges particles i and j. Without too much details this can be achieved with a linear combination of product states known as a Slater determinant

$$|\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_A\rangle = \frac{1}{\sqrt{A!}} \begin{vmatrix} |\alpha_1\rangle_1 & |\alpha_2\rangle_1 & \cdots & |\alpha_A\rangle_1 \\ |\alpha_1\rangle_2 & |\alpha_2\rangle_2 & \cdots & |\alpha_A\rangle_2 \\ \vdots & \vdots & \ddots & \vdots \\ |\alpha_1\rangle_A & |\alpha_2\rangle_A & \cdots & |\alpha_A\rangle_A \end{vmatrix}. \tag{3.3}$$

There is however a much more efficient notation to write fully antisymmeterized many-body quantum states, known as second quantization. In short one begins by introducing the concept of a vacuum state $|0\rangle$ with no particles, normalized such that $\langle 0|0\rangle = 1$. To add and remove particles, the notion of creation and annihilation operators $c^\dagger_\alpha$ and c_α is introduced. These operators obey the following anticommutation rules

$$\{c_\alpha, c_\beta\} = 0 \tag{3.4}$$
$$\{c^\dagger_\alpha, c^\dagger_\beta\} = 0 \tag{3.5}$$
$$\{c^\dagger_\alpha, c_\beta\} = \delta_{\alpha,\beta}. \tag{3.6}$$

If the annihilation operator is applied directly on the vacuum, the result is zero, $c_\alpha|0\rangle = 0$.
A Slater determinant consisting of A particles can then be written as

$$|\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_A\rangle = c^\dagger_{\alpha_1} c^\dagger_{\alpha_2} \cdots c^\dagger_{\alpha_A} |0\rangle . \tag{3.7}$$

To prove that this state is indeed antisymmetric, consider

$$\begin{aligned} P_{i,j}\left|\alpha_1,\alpha_2,\ldots,\alpha_i,\ldots,\alpha_j,\ldots,\alpha_A\right\rangle =& P_{i,j}c^\dagger_{\alpha_1}c^\dagger_{\alpha_2}\cdots c^\dagger_{\alpha_i}\cdots \\ & c^\dagger_{\alpha_j}\cdots c^\dagger_{\alpha_A}\left|0\right\rangle \\ =& c^\dagger_{\alpha_1}c^\dagger_{\alpha_2}\cdots c^\dagger_{\alpha_{i-1}}c^\dagger_{\alpha_j}c^\dagger_{\alpha_{i+1}}\cdots \\ & c^\dagger_{\alpha_{j-1}}c^\dagger_{\alpha_i}c^\dagger_{\alpha_{j+1}}\cdots c^\dagger_{\alpha_A}\left|0\right\rangle \end{aligned} \tag{3.8}$$

Now I use anticommutator rule (3.5) to move $c^\dagger_i$ close to $c^\dagger_j$. For every creation operator between them there will be a sign change since $\{c^\dagger_\alpha, c^\dagger_\beta\} = c^\dagger_\alpha c^\dagger_\beta + c^\dagger_\beta c^\dagger_\alpha = 0$. There are $j-i-1$ creation operators to pass and I therefore get

$$\begin{aligned} P_{i,j}\left|\alpha_1,\alpha_2,\ldots,\alpha_i,\ldots,\alpha_j,\ldots,\alpha_A\right\rangle =& c^\dagger_{\alpha_1}c^\dagger_{\alpha_2}\cdots c^\dagger_{\alpha_{i-1}}c^\dagger_{\alpha_j}c^\dagger_{\alpha_{i+1}}\cdots \\ & c^\dagger_{\alpha_{j-1}}c^\dagger_{\alpha_i}c^\dagger_{\alpha_{j+1}}\cdots c^\dagger_{\alpha_A}\left|0\right\rangle \\ =& (-1)^{j-i-1}c^\dagger_{\alpha_1}c^\dagger_{\alpha_2}\cdots c^\dagger_{\alpha_{i-1}}c^\dagger_{\alpha_j}c^\dagger_{\alpha_i}c^\dagger_{\alpha_{i+1}}\cdots \\ & c^\dagger_{\alpha_{j-1}}c^\dagger_{\alpha_{j+1}}\cdots c^\dagger_{\alpha_A}\left|0\right\rangle . \end{aligned} \tag{3.9}$$

We can now use anticommutator rule (3.5) again, to swap place on $c^\dagger_{\alpha_i}$ and $c^\dagger_{\alpha_j}$ and get

$$\begin{aligned} P_{i,j}\left|\alpha_1,\alpha_2,\ldots,\alpha_i,\ldots,\alpha_j,\ldots,\alpha_A\right\rangle =& (-1)^{j-i-1}c^\dagger_{\alpha_1}c^\dagger_{\alpha_2}\cdots c^\dagger_{\alpha_{i-1}}c^\dagger_{\alpha_j}c^\dagger_{\alpha_i}c^\dagger_{\alpha_{i+1}}\cdots \\ & c^\dagger_{\alpha_{j-1}}c^\dagger_{\alpha_{j+1}}\cdots c^\dagger_{\alpha_A}\left|0\right\rangle \\ =& (-1)^{j-i}c^\dagger_{\alpha_1}c^\dagger_{\alpha_2}\cdots c^\dagger_{\alpha_{i-1}}c^\dagger_{\alpha_i}c^\dagger_{\alpha_j}c^\dagger_{\alpha_{i+1}}\cdots \\ & c^\dagger_{\alpha_{j-1}}c^\dagger_{\alpha_{j+1}}\cdots c^\dagger_{\alpha_A}\left|0\right\rangle \end{aligned} \tag{3.10}$$

and finally we move $c^\dagger_{\alpha_j}$ to the place between $c^\dagger_{\alpha_{j-1}}$ and $c^\dagger_{\alpha_{j+1}}$ which give us

$$\begin{aligned} P_{i,j}\left|\alpha_1,\alpha_2,\ldots,\alpha_i,\ldots,\alpha_j,\ldots,\alpha_A\right\rangle =& (-1)^{j-i}c^\dagger_{\alpha_1}c^\dagger_{\alpha_2}\cdots c^\dagger_{\alpha_{i-1}}c^\dagger_{\alpha_i}c^\dagger_{\alpha_j}c^\dagger_{\alpha_{i+1}}\cdots \\ & c^\dagger_{\alpha_{j-1}}c^\dagger_{\alpha_{j+1}}\cdots c^\dagger_{\alpha_A}\left|0\right\rangle \\ =& -c^\dagger_{\alpha_1}c^\dagger_{\alpha_2}\cdots c^\dagger_{\alpha_{i-1}}c^\dagger_{\alpha_i}c^\dagger_{\alpha_{i+1}}\cdots \\ & c^\dagger_{\alpha_{j-1}}c^\dagger_{\alpha_j}c^\dagger_{\alpha_{j+1}}\cdots c^\dagger_{\alpha_A}\left|0\right\rangle \\ =& -\left|\alpha_1,\alpha_2,\ldots,\alpha_i,\ldots,\alpha_j,\ldots,\alpha_A\right\rangle . \end{aligned} \tag{3.11}$$

This way of expressing many-body states is very powerful, and is therefore used frequently throughout this thesis. For a more complete discussion on creation and annihilation operators and second quantization I refer the reader to Shavitt and Bartlett [5].

3.1.2 Angular-momentum coupled basis

Now let us take a look at the many-body states with coupled angular momenta. The basic motivation to use a coupled many-body basis is that angular momentum is a conserved quantity in the absence of external influences on the system. By expressing

the interaction in a basis with coupled angular momenta certain redundancies might be eliminated and could result in smaller interaction matrices and save precious memory space on a computer.
In the case of two particles there is a total isospin as well as a total angular momentum. These states are written as

$$|(n_a l_a t_a j_a, n_b l_b t_b j_b) J_{ab} M_{ab} T_{ab} T_{zab}\rangle = |(a t_a j_a, b t_b j_b) J_{ab} M_{ab} T_{ab} T_{zab}\rangle \tag{3.12}$$

or sometimes with single-particle isospin omitted. The indices a and b represent all quantum numbers that are not relevant for the coupling, such as n and l, this notation will occur throughout this thesis. Naturally these states have to be antisymmetrized, which will exclude all states where the single particle quantum numbers are equal and $J_{ab} + T_{ab}$ is an even number, as will be shown in section 3.2.1.
The coupled three-particle case is more involved. Such states are written on the form

$$|((n_a l_a j_a, n_b l_b j_b) J_{ab} n_c l_c j_c) J_{abc} M_{abc}\rangle = |((a j_a, b j_b) J_{ab} c j_c) J_{abc} M_{abc}\rangle \,. \tag{3.13}$$

The indices a,b and c represent also in this case all quantum numbers not relevant for the coupling. We use three-body states that are not coupled in isospin. t and t_z are therefore included in a,b and c.
It is possible to couple the angular momenta of three-particles in different ways. For instance j_a could be coupled to j_b and give J_{ab}, which then could be coupled to j_c forming J_{abc}. However, it is also possible to couple j_b and j_c first and then couple j_a to them. Because of this ambiguity combined with the antisymmetry it turns out that the anti-symmetric coupled three-particle basis must therefore be overcomplete to fully span the Hilbert space.

3.1.3 Energy truncations

It is necessary to truncate the many-body basis to facilitate a computational implementation. Therefore the many-body basis is truncated in total harmonic oscillator energy,

$$N = N_1 + N_2 + N_3 + \cdots + N_A - N_{ground} \leq N_{max}, \tag{3.14}$$

where N_i is the harmonic oscillator quantum number for particle i and N_{ground} is the Fermi level. The dimension of the many-body basis increases with N_{max}. A CI calculation is a variational calculation, therefore increasing N_{max} results in a better approximation.

3.2 Decoupling the matrix elements

It is easier to perform a CI calculation when the matrix elements of the forces are expressed in an m-scheme basis. However, the provided two-body forces and the three-body forces were given in an angular-momentum coupled representation. Furthermore, the isospin of two-body forces is also coupled. In this section I will therefore discuss how to transform the matrix elements from a coupled basis to the m-scheme basis. Both the m-scheme basis and the coupled basis have been discussed in section 3.1, so I will mainly focus on relation between the two in this section.

3.2.1 Decoupling two-body force matrix elements

The matrix elements for the two-body forces are given in a basis where the two particles have coupled angular momenta and coupled isospin,

$$\langle (a't'_a j'_a, b't'_b j'_b) J_{ab} T_{ab} | \, V \, | (at_a j_a, bt_b j_b) J_{ab} T_{ab} \rangle \, . \tag{3.15}$$

In this section the aim is to transform these to the m-scheme basis. In the m-scheme basis the matrix elements look like,

$$\langle a't'_a t'_{za} j'_a m'_a, b't'_b t'_{zb} j'_b m'_b | \, V \, | at_a t_{za} j_a m_a, bt_b t_{zb} j_b m_b \rangle \, . \tag{3.16}$$

I will for the moment ignore that the particles are indistinguishable. The relation between the m-scheme states and states with coupled angular momentum are then

$$|at_a t_{za} j_a m_a, bt_b t_{zb} j_b m_b) = \sum_{J_{ab}} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ m_a+m_b \end{smallmatrix} \right)_{\rm cg} |(at_a t_{za} j_a, bt_b t_{zb} j_b) J_{ab} (m_a + m_b)) \, , \tag{3.17}$$

where I used the Clebsch-Gordan coefficient [6]

$$\left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ m_a+m_b \end{smallmatrix} \right)_{\rm cg} . \tag{3.18}$$

The two-body force matrix elements are not just coupled in angular momentum, but also in isospin and the relation to these elements are therefore

$$\begin{aligned} |at_a t_{za} j_a m_a, bt_b t_{zb} j_b m_b) = \sum_{J_{ab}, T_{ab}} & \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ m_a+m_b \end{smallmatrix} \right)_{\rm cg} \left(\begin{smallmatrix} t_a & t_b \\ t_{za} & t_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ t_{za}+t_{zb} \end{smallmatrix} \right)_{\rm cg} \\ & \times |(at_a j_a, bt_b j_b) T_{ab} (t_{za} + t_{zb}) J_{ab} (m_a + m_b)) \, . \end{aligned} \tag{3.19}$$

So far the calculation has been done assuming that the particles are distinguishable but as mentioned earlier, this is not the case. Due to the fermionic nature of the nucleons the states must be antisymmeterised. This results in two complications: 1) some previously allowed coupled states disappear and 2) it is necessary to introduce a normalization constant. The transformation in equation (3.19) is unitary. Therefore the inverse transformation is

$$\begin{aligned} |(at_a j_a, bt_b j_b) T T_z J_{ab} M) = \sum_{\substack{m_a, m_b \\ t_{za}, t_{zb}}} & \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ M \end{smallmatrix} \right)_{\rm cg} \left(\begin{smallmatrix} t_a & t_b \\ t_{za} & t_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ T_z \end{smallmatrix} \right)_{\rm cg} \\ & |at_a t_{za} j_a m_a, bt_b t_{zb} j_b m_b) \end{aligned} \tag{3.20}$$

I replace $|at_a t_{za} j_a m_a, bt_b t_{zb} j_b m_b)$ with

$$|at_{za} j_a m_a, bt_{zb} j_b m_b \rangle = \frac{1}{\sqrt{2}} (|at_{za} j_a m_a, bt_{zb} j_b m_b) - |bt_{zb} j_b m_b, at_{za} j_a m_a)) \tag{3.21}$$

and assume from now on that t_a and t_b is $1/2$ and therefore suppresed in the following. Further I introduce the normalization constant N. Inspired by equation 3.20 I make the ansatz

$$\begin{aligned} |(aj_a, bj_b) T T_z J_{ab} M \rangle = N \sum_{\substack{m_a, m_b \\ t_{za}, t_{zb}}} & \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ M \end{smallmatrix} \right)_{\rm cg} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t_{za} & t_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ T_z \end{smallmatrix} \right)_{\rm cg} \\ & \times |at_{za} j_a m_a, bt_{zb} j_b m_b \rangle_a \, . \end{aligned} \tag{3.22}$$

By forcing unitary normalization on the states we can obtain N by

$$\begin{aligned}
1 =& \langle (aj_a, bj_b) T_{ab} T_z J_{ab} M | (aj_a, bj_b) T_{ab} T_z J_{ab} M \rangle_a \\
=& N^2 \sum_{\substack{m_a, m_b \\ t_{za}, t_{zb}}} \sum_{\substack{m'_a, m'_b \\ t'_{za}, t'_{zb}}} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ M \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t_{za} & t_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ T_z \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_a & j_b \\ m'_a & m'_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ M \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t'_{za} & t'_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ T_z \end{smallmatrix} \right)_{\mathrm{cg}} \\
& \times \langle a t_{za} j_a m_a, b t_{zb} j_b m_b | a t'_{za} j_a m'_a, b t'_{zb} j_b m'_b \rangle_a \\
=& N^2 \sum_{\substack{m_a, m_b \\ t_{za}, t_{zb}}} \sum_{\substack{m'_a, m'_b \\ t'_{za}, t'_{zb}}} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ M \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t_{za} & t_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ T_z \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_a & j_b \\ m'_a & m'_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ M \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t'_{za} & t'_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ T_z \end{smallmatrix} \right)_{\mathrm{cg}} \\
& \times (\delta_{m_a, m'_a} \delta_{m_b, m'_b} \delta_{t_{za}, t'_{za}} \delta_{t_{zb}, t'_{zb}} - \delta_{a,b} \delta_{j_a, j_b} \delta_{m_a, m'_b} \delta_{m_b, m'_a} \delta_{t_{za}, t'_{zb}} \delta_{t_{zb}, t'_{za}}) \\
=& N^2 \left(\sum_{\substack{m_a, m_b \\ t_{za}, t_{zb}}} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ M \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t_{za} & t_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ T_z \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ M \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t_{za} & t_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ T_z \end{smallmatrix} \right)_{\mathrm{cg}} \right. \\
& \left. - \sum_{\substack{m_a, m_b \\ t_{za}, t_{zb}}} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ M \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t_{za} & t_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ T_z \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_a & j_b \\ m_b & m_a \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ M \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t_{zb} & t_{za} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ T_z \end{smallmatrix} \right)_{\mathrm{cg}} \delta_{a,b} \delta_{j_a, j_b} \right)
\end{aligned} \tag{3.23}$$

The first sum in the last step becomes 1. The second sum becomes $(-1)^{J_{ab}+T_{ab}} \delta_{a,b} \delta_{j_a, j_b}$. Therefore the equation simplifies to

$$1 = N^2 (1 - (-1)^{J_{ab}+T_{ab}} \delta_{a,b} \delta_{j_a, j_b}). \tag{3.24}$$

If $a = b$ and $j_a = j_b$ this equation is only true for $J_{ab} + T_{ab} =$ odd, in which case $N = \frac{1}{\sqrt{2}}$. If $a \neq b$ or $j_a \neq j_b$ then $N = 1$.
Thus the relation between m-scheme matrix elements and the coupled matrix elements must be

$$\begin{aligned}
& \langle a' t'_{za} j'_a m'_a, b' t'_{zb} j'_b m'_b | \, V \, | a t_{za} j_a m_a, b t_{zb} j_b m_b \rangle = \\
& \frac{1}{N N'} \sum_{J_{ab} T_{ab}} \sum_{J'_{ab} T'_{ab}} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ m_a + m_b \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t_{za} & t_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T_{ab} \\ t_{za} + t_{zb} \end{smallmatrix} \right)_{\mathrm{cg}} \\
& \times \left(\begin{smallmatrix} j'_a & j'_b \\ m'_a & m'_b \end{smallmatrix} \middle| \begin{smallmatrix} J'_{ab} \\ m'_a + m'_b \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t'_{za} & t'_{zb} \end{smallmatrix} \middle| \begin{smallmatrix} T'_{ab} \\ t'_{za} + t'_{zb} \end{smallmatrix} \right)_{\mathrm{cg}} \\
& \times \langle (a' j'_a, b' j'_b) J'_{ab} (m'_a + m'_b) T'_{ab} (t'_{za} + t'_{zb}) | \, V \, | (a j_a, b j_b) J_{ab} (m_a + m_b) T_{ab} (t_{za} + t_{zb}) \rangle \, .
\end{aligned} \tag{3.25}$$

Up to this point I have not taken into account possible symmetries of the potential. A physical interaction, like the two-body forces that we are using in this project, is a rank zero tensor. Therefore we can apply the Wigner-Eckart theorem, which states the following

$$\begin{aligned}
& \langle (a' j'_a, b' j'_b) J'_{ab} (m'_a + m'_b) T'_{ab} (t'_{za} + t'_{zb}) | \, V \, | (a j_a, b j_b) J_{ab} (m_a + m_b) T_{ab} (t_{za} + t_{zb}) \rangle = \\
& \left(\begin{smallmatrix} J'_{ab} & 0 \\ (m'_a + m'_b) & 0 \end{smallmatrix} \middle| \begin{smallmatrix} J_{ab} \\ (m_a + m_b) \end{smallmatrix} \right)_{\mathrm{cg}} \langle (a' j'_a, b' j'_b) J'_{ab} T'_{ab} (t'_{za} + t'_{zb}) | \, V \, | (a j_a, b j_b) J_{ab} T_{ab} (t_{za} + t_{zb}) \rangle = \\
& \delta_{J'_{ab}, J_{ab}} \delta_{m'_a + m'_b, m_a + m_b} \langle (a' j'_a, b' j'_b) J'_{ab} T'_{ab} (t'_{za} + t'_{zb}) | \, V \, | (a j_a, b j_b) J_{ab} T_{ab} (t_{za} + t_{zb}) \rangle \, .
\end{aligned} \tag{3.26}$$

The two-body interactions considered here conserve the total isospin projection. The relation between the m-scheme matrix elements and the coupled matrix elements for the two-body force is therefore

$$\begin{aligned}
&\langle a' t'_{za} j'_a m'_a, b' t'_{zb} j'_b m'_b | \, V \, | a t_{za} j_a m_a, b t_{zb} j_b m_b \rangle = \\
&\frac{\delta_{t'_{za}+t'_{zb},t_{za}+t_{zb}}}{NN'} \sum_{J_{ab}T_{ab}} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \, \begin{smallmatrix} J_{ab} \\ m_a+m_b \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t_{za} & t_{zb} \end{smallmatrix} \middle| \, \begin{smallmatrix} T_{ab} \\ t_{za}+t_{zb} \end{smallmatrix} \right)_{\mathrm{cg}} \\
&\times \left(\begin{smallmatrix} j'_a & j'_b \\ m'_a & m'_b \end{smallmatrix} \middle| \, \begin{smallmatrix} J_{ab} \\ m'_a+m'_b \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} 1/2 & 1/2 \\ t'_{za} & t'_{zb} \end{smallmatrix} \middle| \, \begin{smallmatrix} T_{ab} \\ t'_{za}+t'_{zb} \end{smallmatrix} \right)_{\mathrm{cg}} \\
&\times \langle (a' j'_a, b' j'_b) J_{ab} T_{ab} (t_{za} + t_{zb}) | \, V \, | (a j_a, b j_b) J_{ab} T_{ab} (t_{za} + t_{zb}) \rangle \, .
\end{aligned} \tag{3.27}$$

In the program, this is the expression that is used.

3.2.2 Decoupling three-body force matrix elements

In this part I will discuss the decoupling of the three-body force matrix elements that were provided for this project. I will basically follow the same train of thought as with the two-body force matrix elements, however there are a few differences. The most obvious difference is that isospin is not a coupled quantity but this will not really affect the argument.
The coupled matrix elements are on the form

$$\langle ((a' j'_a, b' j'_b) J'_{ab}, c' j'_c) J_{abc} | \, V \, | ((a j_a, b j_b) J_{ab}, c j_c) J_{abc} \rangle \, . \tag{3.28}$$

Just like for the two-body force matrix elements I will for the moment ignore that the particles are indistinguishable fermions and return to that issue further down the line. I will therefore assume that the provided matrix elements are on the form

$$\langle ((a' j'_a, b' j'_b) J'_{ab}, c' j'_c) J_{abc} | \, V \, | ((a j_a, b j_b) J_{ab}, c j_c) J_{abc} \rangle \, . \tag{3.29}$$

The task is to transform these coupled matrix elements into the m-scheme elements

$$\langle \alpha', \beta', \gamma' | \, V \, | \alpha, \beta, \gamma \rangle = \langle a' j'_a m'_a, b' j'_b m'_b, c' j'_c m'_c | \, V \, | a j_a m_a, b j_b m_b, c j_c m_c \rangle \, . \tag{3.30}$$

The first thing to do is to couple all three particles. I begin by coupling particles a and b. It is of course possible to choose any other of the six possible particle pairs, but all possibilities are related via Wigner 6j symbols [6] and therefore span the same Hilbert space. The relationship between the basis states in the m-scheme and with coupled angular momentum for a and b is

$$|a j_a m_a, b j_b m_b, c j_c m_c) = \sum_{\substack{J_{ab}= \\ |j_a - j_b|}}^{j_a+j_b} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \, \begin{smallmatrix} J_{ab} \\ m_a+m_b \end{smallmatrix} \right)_{\mathrm{cg}} |(a j_a, b j_b) J_{ab} m_a + m_b, c j_c m_c) \, . \tag{3.31}$$

The angular momentum for the third particle can be coupled in a similar way with the total angular momentum of the first two (J_{ab}) resulting in

$$|aj_am_a, bj_bm_b, cj_cm_c) = \sum_{\substack{J_{ab}= \\ |j_a-j_b|}}^{j_a+j_b} \sum_{\substack{J_{abc}= \\ |J_{ab}-j_c|}}^{J_{ab}+j_c} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix}\middle| \begin{smallmatrix} J_{ab} \\ m_a+m_b \end{smallmatrix}\right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_{ab} & j_c \\ m_a+m_b & m_c \end{smallmatrix}\middle| \begin{smallmatrix} J_{abc} \\ m_a+m_b+m_c \end{smallmatrix}\right)_{\mathrm{cg}} \times |((aj_a, bj_b)J_{ab}, cj_c)J_{abc}m_a + m_b + m_c) \,. \tag{3.32}$$

The matrix element can therefore be written as

$$\begin{aligned}
&(a'j'_am'_a, b'j'_bm'_b, c'j'_cm'_c|\, V\, |aj_am_a, bj_bm_b, cj_cm_c) = \\
&\sum_{\substack{J'_{ab}= \\ |j'_a-j'_b|}}^{j'_a+j'_b} \sum_{\substack{J_{ab}= \\ |j_a-j_b|}}^{j_a+j_b} \sum_{\substack{J'_{abc}= \\ |J'_{ab}-j'_c|}}^{J'_{ab}+j'_c} \sum_{\substack{J_{abc}= \\ |J_{ab}-j_c|}}^{J_{ab}+j_c} \left(\begin{smallmatrix} j'_a & j'_b \\ m'_a & m'_b \end{smallmatrix}\middle| \begin{smallmatrix} J'_{ab} \\ m'_a+m'_b \end{smallmatrix}\right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix}\middle| \begin{smallmatrix} J_{ab} \\ m_a+m_b \end{smallmatrix}\right)_{\mathrm{cg}} \times \\
&\left(\begin{smallmatrix} j'_{ab} & j'_c \\ m'_a+m'_b & m'_c \end{smallmatrix}\middle| \begin{smallmatrix} J'_{abc} \\ m'_a+m'_b+m'_c \end{smallmatrix}\right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_{ab} & j_c \\ m_a+m_b & m_c \end{smallmatrix}\middle| \begin{smallmatrix} J_{abc} \\ m_a+m_b+m_c \end{smallmatrix}\right)_{\mathrm{cg}} \times \\
&(((a'j'_a, b'j'_b)J'_{ab}, c'j'_c)J'_{abc}m'_a + m'_b + m'_c|\, V\, |((aj_a, bj_b)J_{ab}, cj_c)J_{abc}m_a + m_b + m_c) \,.
\end{aligned} \tag{3.33}$$

So far no symmetries or features of the potential V have been taken into account. With the same symmetry argument as for two-body forces I can apply the Wigner-Eckart theorem, which yields in this case

$$\begin{aligned}
&(((a'j'_a, b'j'_b)J'_{ab}, c'j'_c)J'_{abc}m'_a + m'_b + m'_c|\, V\, |((aj_a, bj_b)J_{ab}, cj_c)J_{abc}m_a + m_b + m_c) \\
&= \left(\begin{smallmatrix} J'_{abc} & 0 \\ m'_a+m'_b+m'_c & 0 \end{smallmatrix}\middle| \begin{smallmatrix} J_{abc} \\ m_a+m_b+m_c \end{smallmatrix}\right)_{\mathrm{cg}} (((a'j'_a, b'j'_b)J'_{ab}, c'j'_c)J'_{abc}|\, V\, |((aj_a, bj_b)J_{ab}, cj_c)J_{abc}) \\
&= \delta_{J'_{abc},J_{abc}}\delta_{m'_a+m'_b+m'_c,m_a+m_b+m_c} (((a'j'_a, b'j'_b)J'_{ab}, c'j'_c)J'_{abc}|\, V\, |((aj_a, bj_b)J_{ab}, cj_c)J_{abc}) \,.
\end{aligned} \tag{3.34}$$

I can use one Kronecker delta to remove one summation and the final relation is

$$\begin{aligned}
&(a'j'_am'_a, b'j'_bm'_b, c'j'_cm'_c|\, V\, |aj_am_a, bj_bm_b, cj_cm_c) = \\
&\sum_{J'_{ab}} \sum_{J_{ab}} \sum_{J_{abc}} \left(\begin{smallmatrix} j'_a & j'_b \\ m'_a & m'_b \end{smallmatrix}\middle| \begin{smallmatrix} J'_{ab} \\ m'_a+m'_b \end{smallmatrix}\right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix}\middle| \begin{smallmatrix} J_{ab} \\ m_a+m_b \end{smallmatrix}\right)_{\mathrm{cg}} \times \\
&\left(\begin{smallmatrix} j'_{ab} & j'_c \\ m'_a+m'_b & m'_c \end{smallmatrix}\middle| \begin{smallmatrix} J_{abc} \\ m'_a+m'_b+m'_c \end{smallmatrix}\right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_{ab} & j_c \\ m_a+m_b & m_c \end{smallmatrix}\middle| \begin{smallmatrix} J_{abc} \\ m_a+m_b+m_c \end{smallmatrix}\right)_{\mathrm{cg}} \times \\
&\delta_{m'_a+m'_b+m'_c,m_a+m_b+m_c} (((a'j'_a, b'j'_b)J'_{ab}, c'j'_c)J_{abc}|\, V\, |((aj_a, bj_b)J_{ab}, cj_c)J_{abc}) \,.
\end{aligned} \tag{3.35}$$

So far the problem of antisymmeterization has been ignored for the sake of simplicity. It is possible to obtain a normailzation constant analogous to the one obtained for two particles. In a similar way as for the two-body force I make the ansatz

$$\begin{aligned}
|((aj_a, bj_b)J_{ab}, cj_c)J_{abc}M_{abc}\rangle_a =& N \sum_{m_a,m_b,m_c} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix}\middle| \begin{smallmatrix} J_{ab} \\ m_a+m_b \end{smallmatrix}\right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_{ab} & j_c \\ m_a+m_b & m_c \end{smallmatrix}\middle| \begin{smallmatrix} J_{abc} \\ m_a+m_b+m_c \end{smallmatrix}\right)_{\mathrm{cg}} \\
&\times |aj_am_a, bj_bm_b, cj_cm_c\rangle_a \,.
\end{aligned} \tag{3.36}$$

From this ansatz it is possible to show that

$$\begin{aligned}
1 = N^2(1 &+ (-1)^{J_{ab}} \\
&+ (-1)^{j_a+j_b+j_c+J_{abc}}(2J_{ab}+1) \left\{\begin{smallmatrix} j_a & j_b & J_{ab} \\ j_c & j_{abc} & J_{ab} \end{smallmatrix}\right\} \\
&\times (2\delta_{a,b}\delta_{b,c}\delta_{j_a,j_b}\delta_{j_b,j_c} - (-1)^{J_{ab}-j_a-j_b}(\delta_{a,c}\delta_{j_a,j_c} + \delta_{b,c}\delta_{j_b,j_c})))
\end{aligned} \tag{3.37}$$

where $\left\{ \begin{smallmatrix} j_a & j_b & J_{ab} \\ j_c & j_{abc} & J_{ab} \end{smallmatrix} \right\}$ is a Wigner 6j symbol. The derivation is quite tedious but analogous to the method used for two particles and since it turned out that this factor was already included in the matrix elements provided to me, I leave it out of this discussion.
The final expression, including the normalization is therefore

$$\begin{aligned}
&\langle a' j'_a m'_a, b' j'_b m'_b, c' j'_c m'_c | \, V \, | a j_a m_a, b j_b m_b, c j_c m_c \rangle = \\
&\frac{1}{NN'} \sum_{J'_{ab}} \sum_{J_{ab}} \sum_{J_{abc}} \left(\begin{smallmatrix} j'_a & j'_b \\ m'_a & m'_b \end{smallmatrix} \middle| \, \begin{smallmatrix} J'_{ab} \\ m'_a+m'_b \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_a & j_b \\ m_a & m_b \end{smallmatrix} \middle| \, \begin{smallmatrix} J_{ab} \\ m_a+m_b \end{smallmatrix} \right)_{\mathrm{cg}} \times \\
&\left(\begin{smallmatrix} j'_{ab} & j'_c \\ m'_a+m'_b & m'_c \end{smallmatrix} \middle| \, \begin{smallmatrix} J_{abc} \\ m'_a+m'_b+m'_c \end{smallmatrix} \right)_{\mathrm{cg}} \left(\begin{smallmatrix} j_{ab} & j_c \\ m_a+m_b & m_c \end{smallmatrix} \middle| \, \begin{smallmatrix} J_{abc} \\ m_a+m_b+m_c \\ \times \end{smallmatrix} \right)_{\mathrm{cg}} \\
&\delta_{m'_a+m'_b+m'_c, m_a+m_b+m_c} \, \langle ((a' j'_a, b' j'_b) J'_{ab}, c' j'_c) J_{abc} | \, V \, | ((a j_a, b j_b) J_{ab}, c j_c) J_{abc} \rangle \, .
\end{aligned} \tag{3.38}$$

This is the expression used in the software implementation of the decoupling algorithm.

3.3 Three-body matrix elements for identical fermions

In this section I take a look at how three-body force behaves in an $A \geq 3$ body system. I will therefore assume the existence of three-body force elements $V^{\alpha'\beta'\gamma'}_{\alpha\,\beta\,\gamma} = \langle \alpha', \beta', \gamma' | \, V \, | \alpha, \beta, \gamma \rangle$ in a three-body m-scheme basis, where α, β and γ represents relevant single-particle quantum numbers. The task is therefore to express three-body force element in this A body system.
The three-body force term in the A body Hamiltonian can be written as

$$H_{3N} = \sum_{\substack{\alpha\,,\beta\,,\gamma \\ \alpha',\beta',\gamma'}} V^{\alpha'\beta'\gamma'}_{\alpha\,\beta\,\gamma} c^\dagger_{\alpha'} c^\dagger_{\beta'} c^\dagger_{\gamma'} c_\alpha c_\beta c_\gamma . \tag{3.39}$$

where α, β, γ, α', β' and γ' each span all single particle states in the Hilbert space discussed in section 3.1.
To use this in the program, it is required to find non-vanishing matrix elements

$$(H_{3N})_{x,y} = \langle \psi_x | \, H_{3N} \, | \psi_y \rangle \tag{3.40}$$

in the harmonic oscillator basis, discussed in section 3.1. As we saw these basis states can be written using the notation of second quantization

$$|\psi_x\rangle = |\alpha_{x1}, \alpha_{x2}, \ldots, \alpha_{x,A}\rangle = c^\dagger_{\alpha_{x,1}} c^\dagger_{\alpha_{x,2}} \cdots c^\dagger_{\alpha_{x,A}} |0\rangle \, . \tag{3.41}$$

Using this notation, the matrix element becomes.

$$(H_{3N})_{xy} = \langle 0 | \, c_{\alpha_{x,A}} \cdots c_{\alpha_{x,1}} \sum_{\substack{\alpha\,,\beta\,,\gamma \\ \alpha',\beta',\gamma'}} V^{\alpha'\beta'\gamma'}_{\alpha\,\beta\,\gamma} c^\dagger_{\alpha'} c^\dagger_{\beta'} c^\dagger_{\gamma'} c_\alpha c_\beta c_\gamma c^\dagger_{\alpha_{y,1}} \cdots c^\dagger_{\alpha_{y,A}} |0\rangle \tag{3.42}$$

For most choices of $|\psi_x\rangle$ and $|\psi_y\rangle$ this element vanishes, namely all cases where more than three $\alpha_{x,i}$ differ from all $\alpha_{y,j}$. The most obvious case when this element does

not vanish is when the two states are the same, $x = y$. The two cases when one or two $\alpha_{x,i}$ differ from all $\alpha_{y,j}$ can be seen as effective two particle interactions and will also be treated later.
The last remaining case of non vanishing $(H_{3N})_{xy}$ is when exactly three $\alpha_{x,i}$ differ from all $\alpha_{y,j}$. More precisely this means that there exists i_1, i_2, i_3 such that there exsits no j for which $\alpha_{x,i_k} = \alpha_{y,j}$.
Due to that the Pauli exclusion principle assures as that each single particle quantum number can only exist once there must exist j_1, j_2, j_3 such that there exists no i for which $\alpha_{y,j_k} = \alpha_{x,i}$. With out loss of generality it is allowed to assume that $i_1 < i_2 < i_3$ and $j_1 < j_2 < j_3$. Using this it is possible to move out the three interesting creation operators in $|\psi_x\rangle$ as follows.

$$\begin{aligned}
|\psi_x\rangle =& c^\dagger_{\alpha_{x,1}} \cdots c^\dagger_{\alpha_{x,i_1}} \cdots c^\dagger_{\alpha_{x,i_2}} \cdots c^\dagger_{\alpha_{x,i_3}} \cdots c^\dagger_{\alpha_{x,A}} |0\rangle \\
=& (-1)^{i_1-1} c^\dagger_{\alpha_{x,i_1}} c^\dagger_{\alpha_{x,1}} \cdots c^\dagger_{\alpha_{x,i_1-1}} c^\dagger_{\alpha_{x,i_1+1}} \cdots c^\dagger_{\alpha_{x,i_2}} \cdots c^\dagger_{\alpha_{x,i_3}} \cdots c^\dagger_{\alpha_{x,A}} |0\rangle \\
=& (-1)^{i_1+i_2-3} c^\dagger_{\alpha_{x,i_1}} c^\dagger_{\alpha_{x,i_2}} c^\dagger_{\alpha_{x,1}} \cdots c^\dagger_{\alpha_{x,i_1-1}} c^\dagger_{\alpha_{x,i_1+1}} \cdots c^\dagger_{\alpha_{x,i_2-1}} c^\dagger_{\alpha_{x,i_2+1}} \cdots \\
& \qquad \cdots c^\dagger_{\alpha_{x,i_3}} \cdots c^\dagger_{\alpha_{x,A}} |0\rangle \\
=& (-1)^{i_1+i_2+i_3-6} c^\dagger_{\alpha_{x,i_1}} c^\dagger_{\alpha_{x,i_2}} c^\dagger_{\alpha_{x,i_3}} c^\dagger_{\alpha_{x,1}} \cdots c^\dagger_{\alpha_{x,i_1-1}} c^\dagger_{\alpha_{x,i_1+1}} \cdots c^\dagger_{\alpha_{x,i_2-1}} c^\dagger_{\alpha_{x,i_2+1}} \cdots \\
& \qquad \cdots c^\dagger_{\alpha_{x,i_3-1}} c^\dagger_{\alpha_{x,i_3+1}} \cdots c^\dagger_{\alpha_{x,A}} |0\rangle \\
=& (-1)^{i_1+i_2+i_3} c^\dagger_{\alpha_{x,i_1}} c^\dagger_{\alpha_{x,i_2}} c^\dagger_{\alpha_{x,i_3}} |\Phi_{x,y}\rangle
\end{aligned} \tag{3.43}$$

where $|\Phi_{x,y}\rangle$ are a manybody state containing all creation operators common to both $|\psi_x\rangle$ and $|\psi_y\rangle$.
In exactly the same way we get that

$$|\psi_y\rangle = (-1)^{j_1+j_2+j_3} c^\dagger_{\alpha_{y,j_1}} c^\dagger_{\alpha_{y,j_2}} c^\dagger_{\alpha_{y,j_3}} |\Phi_{y,x}\rangle \,. \tag{3.44}$$

$|\Phi_{x,y}\rangle$ and $|\Phi_{y,x}\rangle$ must contain the same creation operators. Imposing also that the single particle states are ordered in the same way it follows that

$$|\Phi_{b,a}\rangle = |\Phi_{a,b}\rangle \,. \tag{3.45}$$

All of this reduces to

$$\begin{aligned}
(H_{3N})_{x,y} =& (-1)^{i_1+i_2+i_3+j_1+j_2+j_3} \langle \Phi_{x,y}| \\
& \times c_{\alpha_{x,i_3}} c_{\alpha_{x,i_2}} c_{\alpha_{x,i_1}} \sum_{\substack{\alpha,\beta,\gamma \\ \alpha',\beta',\gamma'}} V^{\alpha'\beta'\gamma'}_{\alpha\,\beta\,\gamma} c^\dagger_{\alpha'} c^\dagger_{\beta'} c^\dagger_{\gamma'} c_\alpha c_\beta c_\gamma c^\dagger_{\alpha_{y,j_1}} c^\dagger_{\alpha_{y,j_2}} c^\dagger_{\alpha_{y,j_3}} \\
& \times |\Phi_{y,x}\rangle
\end{aligned} \tag{3.46}$$

The three annihilation operators to the left, anti-commute with the three creation operators to the right because of the assumptions earlier. Therefore for this to be nonzero only the three creation operators $c^\dagger_{\alpha'} c^\dagger_{\beta'} c^\dagger_{\gamma'}$ can have nonzero anti-commutators with the annihilation operators $c_{\alpha_{x,i_3}} c_{\alpha_{x,i_2}} c_{\alpha_{x,i_1}}$. There are 3! ways to contract these operators, and the sign changes every time on annihilation operators passes through a creation operator. This can be represented using the fully

anti-symmetric three dimensional Levi-Civita symbol. The same way of reasoning can be applied on the three annihilation operators $c_\alpha c_\beta c_\gamma$ and therefore the matrix elements becomes

$$(H_{3N})_{x,y} = (-1)^{i_1+i_2+i_3+j_1+j_2+j_3} \sum_{\substack{k\,,l\,,m \\ k',l',m'}} \epsilon_{k,l,m}\epsilon_{k',l',m'} V^{\alpha_{x,i_k}\alpha_{x,i_l}\alpha_{x,i_m}}_{\alpha_{y,j'_k}\alpha_{y,j'_l}\alpha_{y,j'_m}}. \tag{3.47}$$

So far the properties of $V^{\alpha'\beta'\gamma'}_{\alpha\,\beta\,\gamma}$ have not been discussed. Since the definition is

$$V^{\alpha'\beta'\gamma'}_{\alpha\,\beta\,\gamma} = \langle \alpha'\beta'\gamma' | \, V_{3N} \, | \alpha\beta\gamma \rangle \tag{3.48}$$

where $|\alpha\beta\gamma\rangle$ and $|\alpha'\beta'\gamma'\rangle$ must be fully antisymmeterized fermionic Slater determinants this matrix elements must be antisymmetric in $\alpha\ \beta\ \gamma$ and $\alpha'\beta'\gamma$. Therefore it is allowed to choose a order of i_1, i_2, i_3 and j_1, j_2, j_3 numerically and each Levi-Civita symbol yields a factor 3!. Therefore the three body interaction elements for two states that differs with exactly three particles can be written as

$$(H_{3N})_{x,y} = 36(-1)^{i_1+i_2+i_3+j_1+j_2+j_3} V^{\alpha_{x,i_1}\alpha_{x,i_2}\alpha_{x,i_3}}_{\alpha_{y,j_1}\alpha_{y,j_2}\alpha_{b,j_3}}. \tag{3.49}$$

As mentioned before there are two other cases that need to be considered. The case when the two states are the same, and when the two states differ with one or two particles. In the first case, when the two states are the same, it turns out that three annihiliation operators to the left in equation (3.42) can be picked at random to contract with the creation operators in H_{3N} . The corresponding creation operators to the right must then be contracted with the annihilation operators in H_{3N}. Just as in the case when the states differed with exactly with three fermions, there are 3! ways for the three picked annihilation operators to act on H_{3N},resulting in Levi-Civita symbols and the same for the three creation operators. Because of the anti-symmetric properties of $V^{\alpha'\beta'\gamma'}_{\alpha\,\beta\,\gamma}$ as seen before the Levi-Civita symbols can be replaced by $3!^2$. Hence in this case the matrix elements becomes

$$(H_{3N})_{x,x} = 36 \sum_{i=1}^{A-2} \sum_{j=i+1}^{A-1} \sum_{k=j+1}^{A} V^{\alpha_{x,i}\alpha_{x,j}\alpha_{x,k}}_{\alpha_{x,i}\alpha_{x,j}\alpha_{x,k}} \tag{3.50}$$

The remaining case, when the two states differ with either one or two particles, can be deduced in similar ways as the two cases above. For the case when two particles differ in the state, it is possible to assume that the two out of place particles in state $|\psi_x\rangle$ has the posistions i_1 and i_2, $i_1 < i_2$, and the two out of place particles in $|\psi_y\rangle$ at positions j_1 and j_2. Just as in the case when the states differed with three particles, they can be written as

$$|\psi_x\rangle = |\alpha_{x,1} \ldots \alpha_{x,i_1} \ldots \alpha_{x,i_2} \ldots \alpha_{x,A}\rangle = (-1)^{i_1+i_2-1} c^\dagger_{\alpha_{x,i_1}} c^\dagger_{\alpha_{x,i_2}} |\Phi_{x,y}\rangle \tag{3.51}$$

$$|\psi_y\rangle = |\alpha_{y,1} \ldots \alpha_{y,j_1} \ldots \alpha_{y,j_2} \ldots \alpha_{y,A}\rangle = (-1)^{j_1+j_2-1} c^\dagger_{\alpha_{b,j_1}} c^\dagger_{\alpha_{b,j_2}} |\Phi_{x,y}\rangle \tag{3.52}$$

where

$$\begin{aligned} |\Phi_{x,y}\rangle &= |\alpha_{x,1} \ldots \alpha_{x,i_1-1}\alpha_{x,i_1+1} \ldots \alpha_{x,i_2-1}\alpha_{x,i_2+1} \ldots \alpha_{x,A}\rangle \\ &= |\alpha_{y,1} \ldots \alpha_{y,j_1-1}\alpha_{y,j_1+1} \ldots \alpha_{y,j_2-1}\alpha_{y,j_2+1} \ldots \alpha_{y,A}\rangle . \end{aligned} \tag{3.53}$$

When applying this to equation (3.42), it is clear that after $c_{\alpha_{x,i_1}} c_{\alpha_{x,i_2}}$ and $c^\dagger_{\alpha_{y,j_1}} c^\dagger_{\alpha_{y,j_2}}$ acted on the potential, on creation and on annihilation operator in the potential remains. Therefore one annihilation operator in $\langle \Phi_{x,y}|$ and one creation operator in $|\Phi_{x,y}\rangle$ must act on the potential, and they have to have the same single particle quantum number. All this yields that

$$(H_{3N})_{x,y} = 36(-1)^{i_1+i_2+j_1+j_2} \sum_{\substack{i=1 \\ i\neq i_1, i\neq i_2}}^{A} V^{\alpha_{x,i_1}\alpha_{x,i_2}\alpha_{x,i}}_{\alpha_{y,j_1}\alpha_{y,j_2}\alpha_{x,i}}. \tag{3.54}$$

The same way of resoning can be applied to the situation when the two states differ with only one particle, at position i_1 in $|\psi_x\rangle$ and at j_1 $|\psi_y\rangle$. In this case the matrix element becomes

$$(H_{3N})_{x,y} = 36(-1)^{i_1+j_1} \sum_{\substack{i=1 \\ i\neq i_1}}^{A-1} \sum_{\substack{j=i+1 \\ j\neq i_1}}^{A} V^{\alpha_{x,i_1}\alpha_{x,i}\alpha_{x,j}}_{\alpha_{y,j_1}\alpha_{x,i}\alpha_{x,j}}. \tag{3.55}$$

In both of these two last cases, it might be redundant to exclude the $i = i_1$ terms since if it is assumed that the matrix elements $V^{\alpha'\beta'\gamma'}_{\alpha\,\beta\,\gamma}$ are fully antisymmetric in the indices, they have to be zero if two indices are the same.

3.4 Encoding two-body forces in a three-body basis

The Hamiltonian corresponding to a two-body force can be written using second quantization as

$$H_{2N} = \frac{1}{2} \sum_{\substack{\alpha\,,\beta \\ \alpha',\beta'}} V_{2N}{}^{\alpha\,\beta}_{\alpha'\beta'} c^\dagger_\alpha c^\dagger_\beta c_{\beta'} c_{\alpha'}, \tag{3.56}$$

where $V_{2N}{}^{\alpha\,\beta}_{\alpha'\beta'}$ is the two body matrix element, assumed to be antisymmetric in α, β (α', β'). [5]
We can consider the some operator evaluated in a three-body basis,

$$\begin{aligned} V^{\alpha'_1,\alpha'_2,\alpha'_3}_{\alpha_1,\alpha_2,\alpha_3} &= \langle \alpha'_1, \alpha'_2, \alpha'_3 | H_{2N} | \alpha_1, \alpha_2, \alpha_3 \rangle = \\ &\frac{1}{2} \langle 0 | c_{\alpha'_3} c_{\alpha'_2} c_{\alpha'_1} \sum_{\substack{\alpha\,,\beta \\ \alpha',\beta'}} V_{2N}{}^{\alpha\,\beta}_{\alpha'\beta'} c^\dagger_\alpha c^\dagger_\beta c_{\beta'} c_{\alpha'} c^\dagger_{\alpha_1} c^\dagger_{\alpha_2} c^\dagger_{\alpha_3} | 0 \rangle . \end{aligned} \tag{3.57}$$

From the anticommutation rules of the creation and annihilation operators it follows that

$$\begin{aligned} V^{\alpha'_1,\alpha'_2,\alpha'_3}_{\alpha_1,\alpha_2,\alpha_3} = 2(& V_{2N}{}^{\alpha'_1\alpha'_2}_{\alpha_1\alpha_2} \delta^{\alpha'_3}_{\alpha_3} + V_{2N}{}^{\alpha'_3\alpha'_1}_{\alpha_1\alpha_2} \delta^{\alpha'_2}_{\alpha_3} + V_{2N}{}^{\alpha'_2\alpha'_3}_{\alpha_1\alpha_2} \delta^{\alpha'_1}_{\alpha_3} \\ & + V_{2N}{}^{\alpha'_1\alpha'_2}_{\alpha_3\alpha_1} \delta^{\alpha'_3}_{\alpha_2} + V_{2N}{}^{\alpha'_3\alpha'_1}_{\alpha_3\alpha_1} \delta^{\alpha'_2}_{\alpha_2} + V_{2N}{}^{\alpha'_2\alpha'_3}_{\alpha_3\alpha_1} \delta^{\alpha'_1}_{\alpha_2} \\ & + V_{2N}{}^{\alpha'_1\alpha'_2}_{\alpha_2\alpha_3} \delta^{\alpha'_3}_{\alpha_1} + V_{2N}{}^{\alpha'_3\alpha'_1}_{\alpha_2\alpha_3} \delta^{\alpha'_2}_{\alpha_1} + V_{2N}{}^{\alpha'_2\alpha'_3}_{\alpha_2\alpha_3} \delta^{\alpha'_1}_{\alpha_1}), \end{aligned} \tag{3.58}$$

where I have used the assumed antisymmetry in the indices of V_{2N}.
The naive way to construct a three body operator from this would be

$$\hat{O}_{3N} = \frac{1}{6} \sum_{\substack{\alpha,\beta,\gamma \\ \alpha',\beta',\gamma'}} V^{\alpha\beta\gamma}_{\alpha'\beta'\gamma'} c^\dagger_\alpha c^\dagger_\beta c^\dagger_\gamma c_{\gamma'} c_{\beta'} c_{\alpha'}. \tag{3.59}$$

However, there is a problem with this operator as seen when trying to express it in terms of H_{2N},

$$\begin{aligned}
\hat{O}_{3N} &= \frac{1}{6} \sum_{\substack{\alpha,\beta,\gamma \\ \alpha',\beta',\gamma'}} V^{\alpha\beta\gamma}_{\alpha'\beta'\gamma'} c^\dagger_\alpha c^\dagger_\beta c^\dagger_\gamma c_{\gamma'} c_{\beta'} c_{\alpha'} \\
&= \frac{1}{3} \sum_{\substack{\alpha,\beta,\gamma \\ \alpha',\beta',\gamma'}} (V_{2N}{}^{\alpha\beta}_{\alpha'\beta'} \delta^\gamma_{\gamma'} + V_{2N}{}^{\gamma\alpha}_{\alpha'\beta'} \delta^\beta_{\gamma'} + V_{2N}{}^{\beta\gamma}_{\alpha'\beta'} \delta^\alpha_{\gamma'} \\
&+ V_{2N}{}^{\alpha\beta}_{\gamma'\alpha'} \delta^\gamma_{\beta'} + V_{2N}{}^{\alpha\beta}_{\gamma'\alpha'} \delta^\beta_{\beta} + V_{2N}{}^{\beta\gamma}_{\gamma'\alpha'} \delta^\alpha_{\beta'} \\
&+ V_{2N}{}^{\alpha\beta}_{\beta'\gamma'} \delta^\gamma_{\alpha'} + V_{2N}{}^{\gamma\alpha}_{\beta'\gamma'} \delta^\beta_{\alpha'} + V_{2N}{}^{\beta\gamma}_{\beta'\gamma'} \delta^\alpha_{\alpha'}) c^\dagger_\alpha c^\dagger_\beta c^\dagger_\gamma c_{\gamma'} c_{\beta'} c_{\alpha'} \\
&= 3 \sum_{\substack{\alpha,\beta,\gamma \\ \alpha',\beta',\gamma'}} V_{2N}{}^{\alpha\beta}_{\alpha'\beta'} \delta^\gamma_{\gamma'} c^\dagger_\alpha c^\dagger_\beta c^\dagger_\gamma c_{\gamma'} c_{\beta'} c_{\alpha'} \\
&= 3 \sum_{\substack{\alpha,\beta \\ \alpha',\beta'}} V_{2N}{}^{\alpha\beta}_{\alpha'\beta'} c^\dagger_\alpha c^\dagger_\beta \sum_\gamma c^\dagger_\gamma c_\gamma c_{\beta'} c_{\alpha'} \\
&= 3 \sum_{\substack{\alpha,\beta \\ \alpha',\beta'}} V_{2N}{}^{\alpha\beta}_{\alpha'\beta'} c^\dagger_\alpha c^\dagger_\beta c_{\beta'} c_{\alpha'} \left(\sum_\gamma c^\dagger_\gamma c_\gamma - 2 \right) \\
&= 6 H_{2N} (\hat{A} - 2),
\end{aligned} \tag{3.60}$$

where $\hat{A} = \sum_\gamma c^\dagger_\gamma c_\gamma$ is the operator that counts the total number of particles in a many-body state. Clearly we need some way to compensate for this. Therefore I introduce the projection operator

$$P_A = \frac{1}{A!} \sum_{\alpha_1,\ldots,\alpha_A} c^\dagger_{\alpha_1} \cdots c^\dagger_{\alpha_A} |0\rangle \langle 0| c_{\alpha_A} \cdots c_{\alpha_1} \tag{3.61}$$

which projects onto the subspace containing A particles. This operator is the elementary operator in the Hilbert space for A particles and acts as the zero operator for all other number of particles.
It is therefore possible to construct the effective three-body force

$$H_{eff,3N} = \sum_{A=3}^{\infty} \frac{P_A}{36(A-2)} \sum_{\substack{\alpha,\beta,\gamma \\ \alpha',\beta',\gamma'}} V^{\alpha\beta\gamma}_{\alpha'\beta'\gamma'} c^\dagger_\alpha c^\dagger_\beta c^\dagger_\gamma c_{\gamma'} c_{\beta'} c_{\alpha'}. \tag{3.62}$$

The projection operator will ensure that the correct normalization is applied given a fixed number of particles. Since the number of particles will remain constant in the simulation, it is sufficient to use

$$H^A_{eff3N} \frac{1}{36(A-2)} \sum_{\substack{\alpha,\beta,\gamma \\ \alpha',\beta',\gamma'}} V^{\alpha\beta\gamma}_{\alpha'\beta'\gamma'} c^\dagger_\alpha c^\dagger_\beta c^\dagger_\gamma c_{\gamma'} c_{\beta'} c_{\alpha'} \tag{3.63}$$

in the final program.

3.5 The Lawson term

A particular problem appears when treating an A-body problem in single-particle coordinates. The center of mass dynamics will affect the spectrum, but we are only interested in the internal dynamics of the nucleus. The handling of this problem is one of the main reasons for the choice of a harmonic-oscillator basis, since it separates the center of mass motion from the internal dynamics [7]. In this case there is an interesting way to remove the center of mass spectrum, by introducing a so called Lawson term to the Hamiltonian. The Lawson term takes the form

$$H_L = \lambda \left(\frac{\vec{P}_{cm}^2}{2m_{cm}} + \frac{m_{cm}\omega^2}{2}\vec{R}_{cm}^2 - \frac{3\hbar\omega}{2} \right). \tag{3.64}$$

As can be seen it is a harmonic oscillator in the center of mass coordinates but with a constant offset to make the ground-state energy equal to zero. By setting the parameter λ to a high value any center mass excitation will be shifted to high energies, and only internal excitations will remain at low energy values.
The Lawson term contains both a single-particle operator and a two-particle operator. To prove this, the center of mass coordinates are defined as

$$\vec{R}_{cm} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i, \quad \vec{P}_{cm} = \sum_{i=1}^{A}\vec{p}_i \tag{3.65}$$

where $\vec{r}_i$ and $\vec{p}_i$ are the position and momentum of particle i. When inserting this in the Hamiltonian above we have

$$\begin{aligned} H_L =& \lambda \left(\frac{\sum_{i=1}^{A}\vec{p}_i^2 + 2\sum_{i<j=1}^{A}\vec{p}_i\cdot\vec{p}_j}{2m_{cm}} + \frac{m_{cm}\omega^2}{2A^2}\left(\sum_{i=1}^{A}\vec{r}_i^2 + 2\sum_{i<j=1}^{A}\vec{r}_i\cdot\vec{r}_j \right) - \frac{3\hbar\omega}{2} \right) \\ =& \lambda \left(\underbrace{\sum_{i=1}^{A}\left(\frac{\vec{p}_i^2}{2m_{cm}} + \frac{m_{cm}\omega^2}{2A^2}\vec{r}_i^2 \right)}_{(a)} + \underbrace{\sum_{i<j=1}^{A}\left(\frac{\vec{p}_i\cdot\vec{p}_j}{m_{cm}} + \frac{m_{cm}\omega^2}{A^2}\vec{r}_i\cdot\vec{r}_j \right)}_{(b)} - \frac{3\hbar\omega}{2} \right). \end{aligned} \tag{3.66}$$

The term (a) do not mix the dynamics of different particles and acts therefore as a one particle operator, while term (b) do mix the dynamics of each pair of particles.

4

The Software

The previous chapter provided an introduction to many-body theory and the second quantization formalism. I discussed, in particular, three-body operators and the evaluation of matrix elements in both angular-momentum coupled and decoupled three-body bases. In this chapter I will focus on the resulting software that was developed in this work. Figure 4.1 contains a flowchart overviewing the different functionalities of this software. In the following I will discuss the various parts and link them to the relevant theory sections in the previous chapter.

4.1 Initialization of different bases

Several different bases are used in this program and need to be initialized. This task corresponds to the theory discussion in 3.1, and to block c) in figure 4.1. Each single-particle (SP) state is represented with a structure containing the integers n, l, j, t_z and m, the SP quantum numbers from 3.1. These states are organized in an array sorted in increasing $N(= 2n + l)$, l, j, t_z and m. The many-body states are a list of indices in the SP state list. The list of many-body basis states is sorted in increasing total N, total T_z, total M, and then lexicographical order of the states.

4.2 Reading of Two-Body Force Matrix Elements

The reading of two-body force matrix elements corresponds to block b) in figure 4.1. The spin-coupled two-body force matrix elements are on the form

$$\langle (a' t'_a j'_a, b' t'_b j'_b) J_{ab} T_{ab} | \, V \, | (a t_a j_a, b t_b j_b) J_{ab} T_{ab} \rangle \,, \tag{3.15}$$

and were provided in two different file formats, a plain-text one and a binary format. I will focus on the plain-text format in the following.
The first row in the matrix-element file contains an integer number n_{tot} giving the total number of matrix elements in the file. The following n_{tot} lines each contain six integers and six fixed-point numbers. The first four integers give the two SP states in the bra and the ket states, then comes the total angular momentum and the total isospin. The fixed-point numbers are the matrix elements: kinetic energy, relative harmonic-oscillator, Coulomb potential, proton-neutron, proton-proton, and neutron-neutron potential.

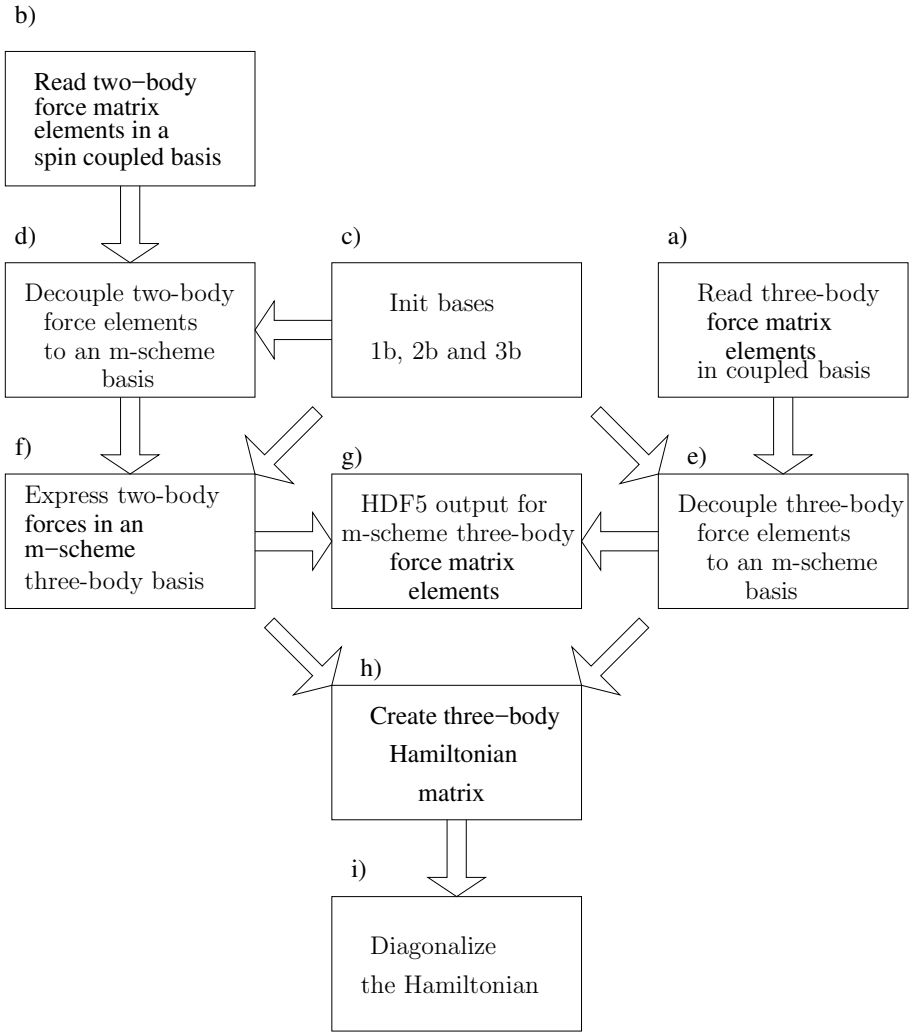

Figure 4.1: Flowchart with the different parts of the program and links between them.

4.3 Spin-Decoupling of Two-Body Matrix Elements

The decoupling of two-body matrix elements in a spin-coupled basis is discussed in theory section 3.2.1. The computational task corresponds to block d) in figure 4.1. The main decoupling is handled in one function, "decouple2B". The function takes two structures as input arguments, one with the coupled matrix element, and the other to tell which coupled matrix elements that is required and containing an array to store the results in.
Two for-loops, one for total J and one for total T, are needed to compute the sum presented in equation (3.27). The two Clebsch-Gordan coefficients for angular-momenta are calculated using

$$\left(\begin{smallmatrix} j_1 & j_2 \\ m_1 & m_2 \end{smallmatrix}\middle| \begin{smallmatrix} J_{12} \\ m_{12} \end{smallmatrix}\right)_{\text{cg}} = \sqrt{2j_{12}+1}(-1)^{j_1-j_2+m_{12}} \left(\begin{smallmatrix} j_1, & j_2 & J_{12} \\ m_1, & m_2 & -m_{12} \end{smallmatrix}\right), \tag{4.1}$$

in which the Wigner-3j symbol on the right-hand side is computed very efficiently with the wigxjpf package [8]. Since the values of the Clebsch-Gordan coefficients

reoccur very frequently they are just computed once and then stored in an array for fast retrieval. The two Clebsch-Gordan coefficients for the coupled iso-spin is trivially either 1 or $\pm 1/\sqrt{2}$. Therefore a conditional statement is used to calculate them.
A hash map is utilized to organize and to look up the coupled two-body force matrix elements and potentially has a near $\mathcal{O}(1)$ behavior.
As an important note, this function also takes care of the one-particle kinetic energy, which is provided as an effective two-body force, and the relative harmonic-oscillator energy (the so called Lawson term) that contains both one- and two-body terms as seen in section 3.5.

4.4 Projection on a Three-Body Basis

The two-body force matrix elements need to be projected on a three-body basis, see section 3.4, to be combined with the three-body force matrix elements that will be read next. This task corresponds to block f) in figure 4.1 and is implemented for two different run modes in the functions "twoBCtoThreeB" and "twoBtoThreeB". Both functions determine which terms in equation 3.58 to use and then apply the normalization discussed at the end of section 3.4. The difference is that "twoBCtoThreeB" calls the decoupling routine discussed in section 4.3 on the fly, while "twoBtoThreeB" uses two-body matrix elements in an m-scheme basis, assuming that the decoupling has been performed in advance.

4.5 Reading of Three-Body Force Matrix Elements

The task of reading three-body force matrix elements from file corresponds to block a) in figure 4.1. The coupled three-body matrix elements are provided as an HDF5 file [9]. Besides the actual matrix elements, the file contains lists over:

- SP states, called "basis", with quantum numbers $n, l, 2j, 2t_z$;
- three-particle states $a, b, c, 2J_{ab}$ called "configurations", where a, b, c are indices for SP states and $2J_{ab}$ is the coupled spin of particles a and b;
- three-particle "channels" $2J_{abc}, 2T_{z,abc}, \Pi_{abc}, 2J_{ab}$ containing conserved quantum numbers.

The number of SP states and configurations are determined from specified energy truncations. The matrix elements,

$$\langle((a'j'_a, b'j'_b)J'_{ab}, c'j'_c)J_{abc}|\, V \,|((aj_a, bj_b)J_{ab}, cj_c)J_{abc}\rangle\,, \tag{3.28}$$

are organised in "data-splits". Each data-split has a corresponding channel and a list of configuration pairs. There might be more channels than data-splits depending on the energy cuts.
For each channel there is an entry for $2J_{ab}$. However, in general this is not a conserved quantity and is not used in this program. Other computational many-body approaches, such as the Coupled-Clusters Method [10], need this.

4.6 Spin-Decoupling of Three-Body Matrix Elements

The implementation of the three-body angular-momentum decoupling, as discussed in theory section 3.2.2, corresponds to block e) in figure 4.1. The angular-momentum decoupling is performed to obtain the matrix elements in m-scheme,

$$\langle \alpha', \beta', \gamma' | \, V \, | \alpha, \beta, \gamma \rangle = \langle a' j'_a m'_a, b' j'_b m'_b, c' j'_c m'_c | \, V \, | a j_a m_a, b j_b m_b, c j_c m_c \rangle \, . \tag{3.30}$$

The function "fCCmatrixElements" takes the two three-particle states $|X\rangle = |\alpha, \beta, \gamma\rangle$ and $|Y\rangle = |\alpha', \beta', \gamma'\rangle$, total isospin projection and total M of the three particles on each side as arguments. The sum in equation (3.38) is divided in three for-loops, one each for J_{ab} and J'_{ab}, and one for J_{abc}. Given the two states $|X\rangle$ and $|Y\rangle$ together with J_{ab}, J'_{ab}, and J_{abc} the function can determine which coupled matrix elements that are needed. Since the input file is organized in different channels, the method "openDataSplit" is used to find the correct channel. It returns a pointer. The channel identification is achieved through a linear search, and might be a focus point for future optimization of the software. When the correct data-split is identified the required coupled matrix element is found by applying the "retriveCoupledMatrixElement" method, which uses a binary search.
There are four Clebsch-Gordan coefficients in equation (3.38). They are calculated with the same routine as in the two-body case.

4.7 HDF5 Output Format

As a bonus feature this software can provide an HDF5 file containing all decoupled three-body matrix. This corresponds to block g) in figure 4.1. The HDF5 file contains, besides the matrix elements, a list of the SP states and a list of three-particle states. The matrix elements are organized in different blocks where all matrix elements have the same total isospin projection and same M quantum number.

4.8 Three-Body Hamiltonian Matrix

The m-scheme matrix elements can now be combined to create the full three-body Hamiltonian matrix, which corresponds to block h) in figure 4.1. This Hamiltonian matrix is then diagonalized in order to solve the Schrödinger equation, corresponding to block i) in figure 4.1. The program applies the lapack routine "dsyev" which diagonalize real symmetric matrices. The resulting eigenspectrum is then stored in a plain-text file with each eigenvalue on a new line.

5
Results

In the two previous chapters the theory of implementing three-body forces in a computer model was addressed. In this section the aim is to verify that the resulting software works correctly. To this end, I compare the calculated ground-state energies for ^{3}H and ^{3}He with experimental as well as theoretical values from Ref. [1].

5.1 Tritium and Helion ground energy

In this section I present the computed ground-state energies E_{gs} of ^{3}H and ^{3}He for different values of N_{max}. I have used NNLOsat [1], a nuclear interaction from chiral-effective field theory with both two- and three-body terms. The results are compared with previously reported calculations [1]. I also extrapolate the calculated ground energies to higher N_{max} by assuming exponential convergence according to

$$E_{\text{gs}}(N_{\text{max}}) = Ae^{-BN_{\text{max}}} + E_{\infty}. \tag{5.1}$$

The value of E_{∞}, is interpreted as the ground energy when $N_{max} \to \infty$.
In table 5.1 and table 5.2 the ground-state energies of ^{3}H and ^{3}He are listed as a function of N_{max}. The values I have calculated are listed under "this work" and the benchmarks values are taken from Ref. [1]. Overall, there is a very small difference of about 1keV between the results from this work and from Ref. [1]. This discrepancy is most likely due to differences in computational code implementation and small deviations in the numerical values of physical constants. Furthermore, the difference in binding energy between ^{3}H and ^{3}He is mostly due to Coulomb effects in ^{3}He.
Already at $N_{\text{max}} = 4$, which constitutes a very small model space, both ^{3}H and ^{3}He receive almost 200keV more binding energy due to the inclusion of a three-body force in the Hamiltonian. At $N_{\text{max}} = 8$ the results are slightly more converged, and the contribution of the three-body force amounts to about 0.5MeV.
To approximate the infinite-space results, i.e. for $N_{\text{max}} \to \infty$, I fit equation (5.1) to the ground-state energies calculated in this work, see tables 5.1 and 5.2.
The resulting functions can be viewed in figure 5.1. The obtained values of E_{∞}, with the inclusion of three-body forces, are -8.560MeV for ^{3}H and -7.793MeV for ^{3}He. These results agree very well with theoretical benchmark values -8.521MeV and -7.765. The measured, ground-state energies of ^{3}H and ^{3}He are -8.482MeV and -7.739MeV [11] respectively.
The extrapolated ground-state energies, for the Hamiltonian without three-body forces, are -7.953MeV for ^{3}H and -7.189MeV for ^{3}He. These values are much

further from the experimental values. This clearly suggests the necessity of three-body forces.

Table 5.1: The ground-state energy, in MeV, for tritium with and without three-body forces.

N_{max}	two-body force		three-body force	
	this work	Ref. [1]	this work	Ref. [1]
0	-0.773654	-0.772807	0.021918	0.022764
2	-3.650272	-3.649317	-3.660361	-3.659447
4	-6.314905	-6.313910	-6.476375	-6.475310
6	-7.383957	-7.383131	-7.810658	-7.809088
8	-7.724727	-7.723948	-8.209156	-8.207927
⋮		⋮		⋮
40		-8.031		-8.521

Table 5.2: The ground-state energy, in MeV, for helion with and without three-body forces.

$N_{\max}$	two-body force only		three-body force	
	this work	Ref. [1]	this work	Ref. [1]
0	0.209011	0.208171	1.004583	1.003742
2	-2.792219	-2.789555	-2.814933	-2.814264
4	-5.489504	-5.487072	-5.659739	-5.657099
6	-6.592230	-6.589451	-7.020912	-7.018062
8	-6.945692	-6.942982	-7.427813	-7.425101
⋮		⋮		⋮
40		-7.282		-7.765

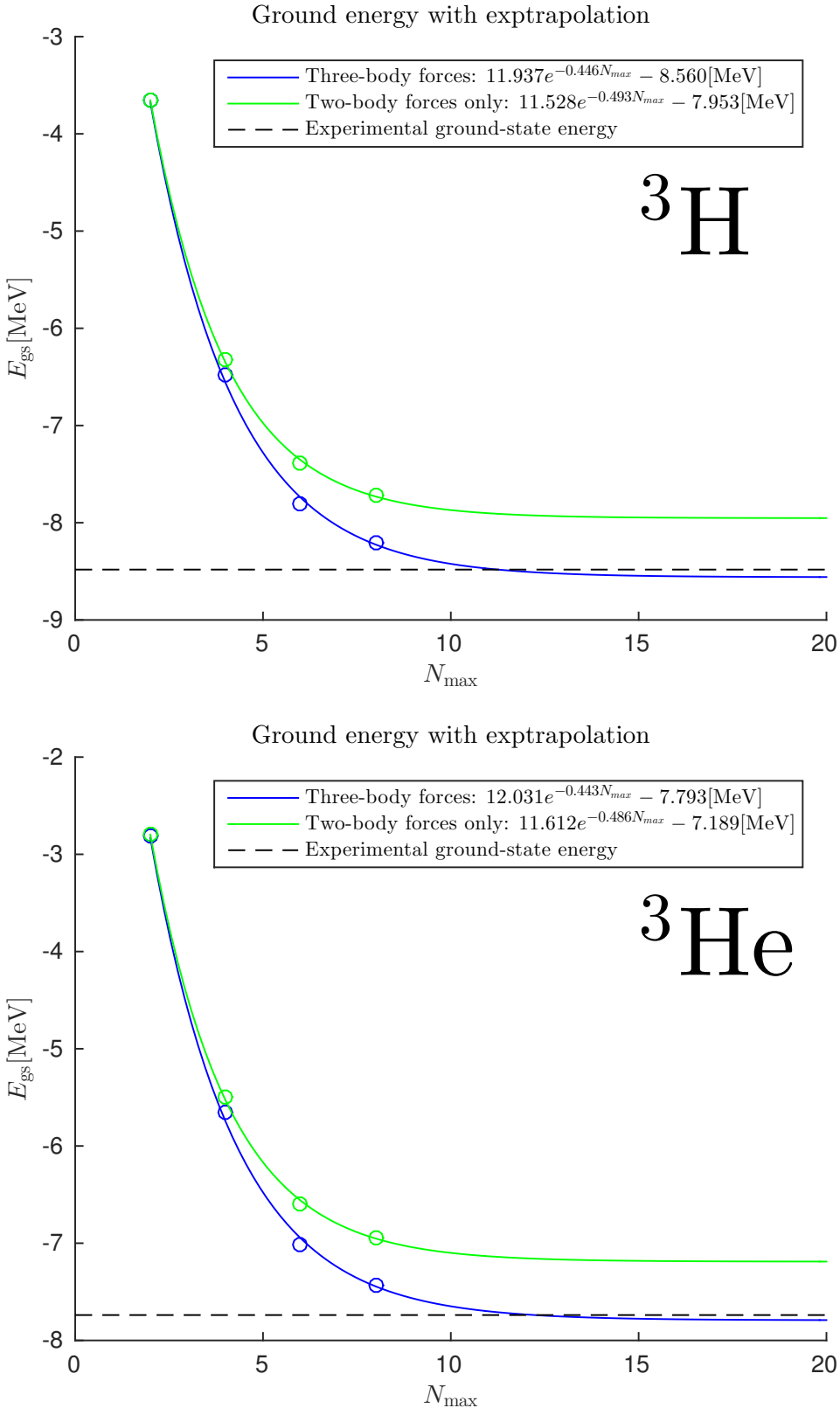

Figure 5.1: The ground-state energies, with three-body forces, as a function of $N_{\max}$ for ^{3}H and ^{3}He. The Blue rings are computed with three-body forces, while the green rings are computed with only two-body forces. The rings are evaluated for $N_{\max} = 2, 4, 6, 8$. The blue and green curves are fitted exponential functions used to extrapolate the ground energies to higher $N_{\max}$, and the dashed line marks the experimental value.

6
Conclusion

Throughout this work the implementation of three-body forces in a quantum many-body configuration-interaction method has been the main focus. As I discussed in the introduction and chapter 2, three-body forces arises in effective theories were the degrees of freedom is reduced. It has been known for a long time that three-body forces are necessary for nuclear physics. This is confirmed by the results presented in chapter 5. The difference between the ground-state energy with and without three-body forces were almost 0.5MeV for $N_{\max} = 8$, which shows a significant effect of the three-body forces. The computed ground-state energy can also be set in contrast with measured values of the ground-state energy for either nuclei, see figure 5.1.
While developing the software, I focused on getting a working program that produced correct results for small systems. Code optimization were only applied when needed, for instance the computation of the Clebsch-Gordan coefficients were terribly slow in the beginning but when reusing earlier calculated coefficients this problem disappeared. However, in the future there will be a demand that the program can handle much bigger model spaces than the present $N_{\max} \leq 8$. This implies that program has to be faster and more memory efficient.
The execution time of the angular-momentum decoupling routine "fCCmatrixElements" have a dependence of the input file size. That is most likely because of the use of a linear search through the channels, and a binary search through the spin-coupled matrix elements, as described in section 4.6. The best way to improve upon this, would be organize all the matrix elements in a hash-map which could reduce access time.
At the moment the program keeps all matrix elements in RAM, which is possible for the model spaces considered throughout this work. However, to obtain fully converged values of the ground-state energy it is necessary to use a model-space with $N_{\max} > 8$. Therefore it would be of future interest to utilize hard-drives to store decoupled matrix elements.
The focus in this work has been on implementing the three-body force elements and therefore the produced software at the moment can only be applied on three-body systems. In the future the aim is to combine this software with a program that can express three-body forces in an A-body basis utilizing the theory in section 3.3.
Since the size of the truncated Hilbert space increases dramatically with the number of particles, it will not be possible to use third party implemented diagonalization routines. This motivate the future implementation of a custome diagonalization routine.

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A

Appendix

A.1 The Harmonic oscillator

The Harmonic Oscillator (HO) is one of the simplest yet useful quantum systems. For this reason it is covered in most standard textbooks on quantum mechanics. Since the choice of basis for the NCSM calculations this project is the eigen states of the HO in three dimensions, it is a good idea to take an additional look at it.
The Hamiltonian of the HO in three dimensions can be written as a particle stuck in quadratic potential,

$$H_{HO} = \frac{\vec{p}^2}{2m} + \frac{m\omega^2}{2} r^2 \tag{A.1}$$

see Sakurai [12].

A.1.1 The wave functions of the Harmonic Oscillator

Even though deriving the wave functions for (A.1) is part of most quantum mechanics textbooks, it still gives a better understanding of the system of doing so. The following derivation is mostly based on the treatment of the problem in Sakurais book [12], but with slight modifications to fit the need of this thesis.
To derive the wavefunctions it is useful to note that the Hamiltonian in (A.1) is spherically symmetric and that the wave functions are separable and can therefore be written as

$$\psi_{n,l,m}(r,\theta,\phi) = \frac{u_{n,l}(r)}{r} Y_{l,m}(\theta,\phi) \tag{A.2}$$

where $Y_{l,m}(\theta,\phi)$ are the ordinary spherical harmonics, and $u_{n,l}(r)$ are to be determined. Using this it is straight forward to see that the time independent Schrödinger equation can be written as

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u_{n,l}(r)}{\partial r^2} + \left(\frac{\hbar^2 l(l+1)}{2mr^2} + \frac{m\omega^2}{2} r^2 - E_{n,l}\right) u_{n,l}(r) = 0 \tag{A.3}$$

where $E_{n,l}$ is the eigen-energy associated with the eigen-state [12]. It is convenient to introduce ρ, $\lambda_{n,l}$ and $\tilde{u}_{n,l}(\rho)$ such that

$$\rho = \sqrt{\frac{m\omega}{h}} r, \quad E_{n,l} = \frac{\hbar\omega}{2}\lambda_{n,l}, \quad \tilde{u}_{n,l}(\rho) = u_{n,l}(r). \tag{A.4}$$

Using this the equation becomes

$$\tilde{u}''_{n,l}(\rho) - \frac{l(l+1)}{\rho^2}\tilde{u}_{n,l}(\rho) + (\lambda_{n,l} - \rho^2)\tilde{u}_{n,l}(\rho) = 0. \tag{A.5}$$

If $l = 0$ this is equation is easy to solve, since the function $\tilde{u}(\rho) = e^{-\frac{\rho^2}{2}}$ would be a solution. An other important realization is when the function $h(\rho) = \rho^{l+1}$ is differentiated twice it becomes $\frac{l(l+1)}{\rho^2}h(\rho)$. In light of this, a reasonable ansatz would be

$$\tilde{u}_{n,l}(\rho) = \rho^{l+1}e^{-\frac{\rho^2}{2}}f_{n,l}(\rho^2). \tag{A.6}$$

where $f_{n,l}(x)$ is a function to be determined The reason for the square of the argument in $f_{n,l}(\rho^2)$ will be apparent when a matching with Laguerre polynomials later on. After some tedious but straight forward algebra, the equation for $f_{n,l}(x)$ becomes

$$4xf''_{n,l}(x) + 2((2l+3) - 2x)f'_{n,l}(x) + (\lambda_{n,l} - (2l+3))f_{n,l}(x) = 0 \tag{A.7}$$

The defining equation for associated Laguerre polynomials are

$$xL''^{k}_{n}(x) + (k+1-x)L'^{k}_{n} + nL^k_n = 0 \tag{A.8}$$

see Mathematical Methods for Physicists [13]. Breaking out a factor of four in equation (A.7) shows that it is the same as (A.8) if $k = l+\frac{1}{2}$ and if $4n = \lambda_{n,l}-(2l+3)$. From this it is clear that

$$f_{n,l}(x) = L_n^{l+1/2}(x), \quad \lambda_{n,l} = 4n + 2l + 3 \tag{A.9}$$

By retracing the steps taken to this point the full wave functions becomes

$$\psi_{n,l,m}(r,\theta,\phi) = A\left(\frac{m\omega}{\hbar}\right)^{\frac{l+1}{2}} r^l e^{-\frac{m\omega}{2\hbar}r^2} L_n^{l+1/2}(\frac{m\omega}{\hbar}r^2)Y_{l,m}(\theta,\phi) \tag{A.10}$$

where A is a normalization constant. The corresponding eigen energy for this states becomes

$$E_{n,l} = \hbar\omega\left(2n + l + \frac{3}{2}\right). \tag{A.11}$$

The normalisation constant can be obtained by

$$1 = \langle n,l,m|n,l,m\rangle = |A|^2\left(\frac{m\omega}{\hbar}\right)^{l+1}\int_0^\infty r^{2l}e^{-\frac{m\omega}{\hbar}r^2}\left(L_n^{l+1/2}\left(\frac{m\omega}{\hbar}r^2\right)\right)^2 r^2dr. \tag{A.12}$$

The integral can be easily evaluated after setting $t = \frac{m\omega}{\hbar}r^2$ using

$$\int_0^\infty t^\alpha e^{-t}L_n^\alpha(t)L_{n'}^\alpha(t) = \frac{\Gamma(n+\alpha+1)}{n!}\delta_{n,n'} \tag{A.13}$$

see Mathematical Methods for Physicists [13], where Γ is the gamma function which yields that

$$1 = \frac{|A|^2}{2}\left(\frac{m\omega}{\hbar}\right)^{-1/2}\frac{\Gamma(n+l+3/2)}{n!}. \tag{A.14}$$

From this we can conclude that

$$A = \sqrt{2\sqrt{\frac{m\omega}{\hbar}}\frac{n!}{\Gamma(n+l+3/2)}} \tag{A.15}$$

(and an arbitrary complex phase which I omit since it is of no relevance in this thesis).