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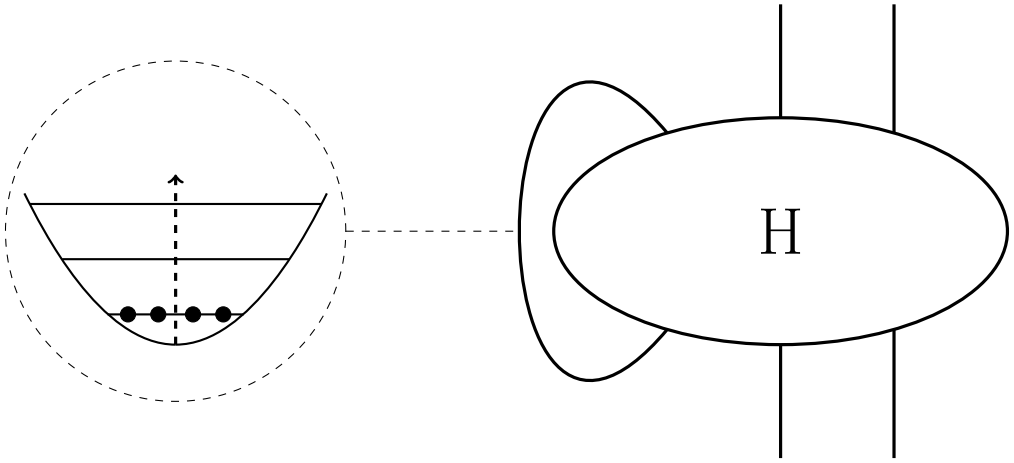

Three-Nucleon Forces Through Normal-Ordered Approximations

Master's thesis in Physics and Astronomy

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Department of Physics
CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden 2016

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Cover: A three-nucleon Hamiltonian is approximated through normal-ordering with respect to a Fermi state.

Typeset in LaTeX
Printed by Chalmers Reproservice
Gothenburg, Sweden 2016

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Abstract

Three-body forces have long been known to play an important role in nuclear physics. However, fully including such interactions in ab-initio methods is computationally expensive and not feasible for larger nuclei. As an alternative, approximations based on normal-ordering with respect to a Fermi state of the nucleus can be used. In this framework part of the three-body interaction can be expressed as lower order interactions, which can be included without increasing the computational complexity. This thesis provides a full derivation of the normal-ordered two-body (NO2B) approximation for closed-shell nuclei. In addition, a simple implementation of this method is described. This is then used to calculate ground states of helium-4 in small model spaces, which are compared to the corresponding calculations with full three-body forces. The results show a relative error of less than 1.5%, in line with earlier studies.

Keywords: ab-initio, nuclear physics, normal-ordered approximation, quantum many-body theory, three-nucleon forces

Acknowledgements

I would like to express my gratitude to the Subatomic Theory group for their hospitality and helpfulness. In particular I would like to thank my two supervisors Andreas Ekström and Christian Forssén for their invaluable assistance, without which this thesis could not have been written. I am also thankful for the many valuable discussions with my fellow master student Tor Djärv.

Dag Fahlin Strömberg, Gothenburg, September 2016

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1
Introduction

The development of precise and efficient ab-initio methods is an important goal in theoretical nuclear physics. Rather than relying on empirical models of the nucleus, such methods start from a microscopic description of the interactions between the individual nucleons. All approximations that are used in these methods are well-controlled and applied in a systematic manner, meaning that the resulting uncertainties can be quantified in a reliable fashion.
A significant challenge in the pursuit of higher accuracy is the inclusion of three-nucleon (3N) interactions. Such interactions arise naturally in Hamiltonians derived from chiral effective field theory [10], which are used as input to most modern ab-initio calculations. Comparisons with experimental data such as [2] have proven that the 3N contribution is not negligible in general.
Fully including 3N interactions in many-body methods is computationally challenging. To see why we must go to the core of the nuclear many-body problem, namely the time-independent Schrödinger equation

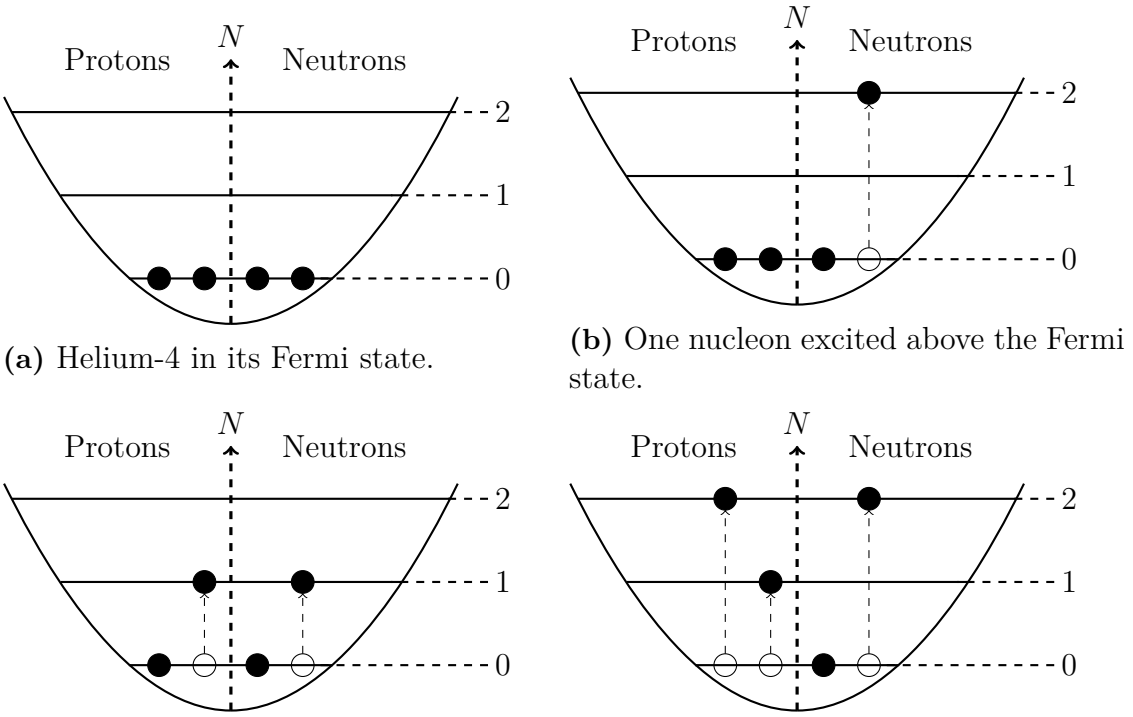
$$H\psi = E\psi, \tag{1.1}$$

where H is a many-body Hamiltonian operator and ψ is a many-body eigenstate. If 3N interactions are included the Hamiltonian operator is

$$H = \sum_{i}^{A} T_i + \sum_{i<j}^{A} V_{ij}^{2N} + \sum_{i<j<k}^{A} V_{ijk}^{3N}, \tag{1.2}$$

where A is the number of nucleons and T_i, V_{ij}^{2N} and V_{ijk}^{3N} represent the kinetic energy, the two-nucleon (2N) interaction and the 3N interaction, respectively. The many-body state ψ exists in a Hilbert space spanned by an infinite basis $\phi_1, \phi_2 \ldots$ This many-body basis is truncated into a finite-sized subset $\phi_1, \phi_2 \ldots \phi_N$, turning (1.1) into a matrix eigenvalue problem. H is replaced by an $N \times N$ matrix given by $(H_N)_{kl} = \langle \phi_k | H | \phi_l \rangle$. For this matrix to be diagonalisable within a reasonable time frame it must be sufficiently sparse, i.e. only a fraction of the elements can be non-zero. We note that the kinetic energy operator is a one-nucleon (1N) operator, meaning that it only affects one nucleon at a time. This implies that the corresponding term in $(H_N)_{kl}$ must be zero if there is more than one single-particle state that does not exist in both ϕ_k and ϕ_l — otherwise there is no 1N operator that can turn the initial state ϕ_l into the final state ϕ_k. In the same fashion, the 2N interaction affects two nucleons simultaneously and only gives non-zero values for $(H_N)_{kl}$ if ϕ_k and ϕ_l have less than two non-shared single-particle states. If the 3N interaction is included as well $(H_N)_{kl}$ can be non-zero for up to three non-shared

single-particle states. This implies that H_N is significantly less sparse if 3N interactions are included. As a consequence of this the computational complexity increases dramatically, especially in larger nuclei.
A compromise between accuracy and computational feasibility can be reached through an approximation scheme. One such approach is the normal-ordered two-body (NO2B) approximation. The underlying idea is to express (normal order) the 3N interaction relative to the Fermi state of the nucleus, i.e. the many-body state where all nucleons occupy the lowest possible single-particle states. This results in an expression for the 3N interaction operator as a sum of a constant (0N), a one-nucleon (1N) operator, a 2N operator and a 3N operator.



(a) Helium-4 in its Fermi state.

(b) One nucleon excited above the Fermi state.

(c) Two nucleons excited above the Fermi state.

(d) Three nucleons excited above the Fermi state.

Figure 1.1: Examples of many-body configurations in a helium-4 nucleus. N is the harmonic oscillator shell number.

To illustrate the meaning of these terms we consider the application of the normal-ordered 3N interaction to the Fermi state of helium-4. The 0N term accounts for all 3N transitions from the Fermi state (shown in Figure 1.1a) to itself. In a similar fashion, the 1N term represents all transitions between the Fermi state and states with one excited nucleon (e.g. 1.1b). The 2N term represents transitions from the Fermi state to states with two excited nucleons (e.g. 1.1c). Finally, the remaining 3N term accounts for all other transitions (such as 1.1d). The normal-ordered 3N interaction can also be applied to other many-body configurations. The 0N, 1N, 2N, and 3N terms then correspond to transitions with three, two, one and zero diagonal single-particle states that belong to the Fermi configuration.
In the NO2B approximation, only the 0N, 1N and 2N terms are retained whereas the

3N term is discarded, allowing us to at least partially account for the 3N interaction without increasing the computational difficulty substantially.
The particular version of normal ordering that is used this thesis is known as single-reference normal ordering. It is valid if a single reference state (the Fermi state) is already a good approximation of the true many-body ground state. This is true for ground states of closed-shell nuclei (such as helium-4).
This thesis aims to provide a full derivation of the NO2B approximation (Chapter 2), describe a simple implementation in Python (Chapter 3), and apply this to ground states of helium-4 in small model spaces (Chapter 4). This is benchmarked against calculations using the full 3N interaction. Finally, a summary of the key points of the thesis as well as an outlook of possible improvements are provided (Chapter 5).

2

Theory

A full derivation of the NO2B approximation can be found in Section 2.2 in this chapter. This adds detail to the more concise derivation previously published in [9]. To provide the reader with the formalism needed to arrive at the NO2B approximation, an introduction to second quantisation and normal ordering is given in Section 2.1. Additional sections on JT-coupling (Section 2.3) and model space truncation (Section 2.4) are also included as a background to the chapters on implementation and results.

2.1 Second Quantisation

Many-body physics is usually expressed in the language of second quantisation. This framework provides a convenient way to describe and manipulate many-body states containing non-fixed numbers of identical particles. An introduction to this subject is included below, and more thorough accounts can be found in textbooks on many-body theory such as [5, 14].

2.1.1 Many-body states

In single-particle quantum mechanics all states exist in a Hilbert space H spanned by basis states $\phi_1, \phi_2, \phi_3, \ldots$ such that any state $\psi \in H$ can be expressed as

$$|\psi\rangle = \sum_i c_i \, |\phi_i\rangle \, .$$

The complex numbers $c_i = \langle\psi|\phi\rangle$ are the projections of ψ on the basis states.
Many-body states exist in product sets of such Hilbert spaces, spanned by products of single-particle basis states. For example, a two-body state can be expressed as a sum of product states such as $\phi_1\phi_2$, $\phi_2\phi_3$, and so on.
In the case of identical particles physical many-body states must also satisfy the spin-statistics theorem. For fermions this means that the state must be anti-symmetric with respect to an interchange of any two particles, i.e.

$$|abc\rangle = - \, |bac\rangle \, .$$

Similarily, boson states must be symmetric under the same transformation. As all nucleons are fermions we will not discuss boson states any further.

Anti-symmetrised states are traditionally constructed as Slater determinants, such as

$$|abc\rangle = \begin{vmatrix} \phi_a(1) & \phi_b(1) & \phi_c(1) \\ \phi_a(2) & \phi_b(2) & \phi_c(2) \\ \phi_a(3) & \phi_b(3) & \phi_c(3) \end{vmatrix} = \phi_a(1)\phi_b(2)\phi_c(3) + \phi_a(3)\phi_b(1)\phi_c(2) + \phi_a(2)\phi_b(3)\phi_c(1) - \phi_a(3)\phi_b(2)\phi_c(1) - \phi_a(2)\phi_b(1)\phi_c(3) - \phi_a(1)\phi_b(3)\phi_c(2).$$

Note that a, b and c above represent the single-particle states occupied by the particles denoted by 1, 2 and 3.

2.1.2 Creation and annihilation operators

In the second quantisation framework many-body states can be modified through the application of *creation* and *annihilation operators*.
To create a particle in the single-particle state p one applies the creation operator $\hat{a}_p^\dagger$

$$\hat{a}_p^\dagger |\rangle = |p\rangle$$

whereas the particle can be removed by the corresponding annihilation operator $\hat{a}_p$

$$\hat{a}_p |p\rangle = |\rangle .$$

Note that $\hat{a}_p^\dagger$ is the Hermitian conjugate of $\hat{a}_p$. The empty ket $|\rangle$ refers to the (physical) vacuum, i.e. a state with zero particles. From this starting point any many-body state can be constructed by applying a sequence of creation operators, e.g.

$$\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r^\dagger |\rangle = \hat{a}_p^\dagger \hat{a}_q^\dagger |r\rangle = \hat{a}_p^\dagger |qr\rangle = |pqr\rangle .$$

If a certain single-particle state is unoccupied, applying the corresponding annihilation operator to the many-body state results in

$$\hat{a}_p |qr\rangle = 0.$$

In other words, one cannot annihilate a particle which does not exist. Due to the Pauli exclusion principle, this also occurs when trying to create a fermion in an already occupied single-particle state

$$\hat{a}_p^\dagger |pqr\rangle = 0.$$

It is important to note that the zeros above simply refer to the number 0 and *not* to the vacuum $|\rangle$.
In the subsequent sections we will need to rearrange products of creation and annihilation operators into certain orders. This reordering can be done by utilising the anti-commutation relations for fermions

$$\{\hat{a}_p, \hat{a}_q^\dagger\} = \hat{a}_p \hat{a}_q^\dagger + \hat{a}_q^\dagger \hat{a}_p = \delta_{p,q} \tag{2.1}$$

$$\{\hat{a}_p, \hat{a}_q\} = 0 \tag{2.2}$$

$$\{\hat{a}_p^\dagger, \hat{a}_q^\dagger\} = 0. \tag{2.3}$$

2.1.3 The Hamiltonian in second quantisation

Second quantisation allows us to express interactions in terms of creation and annihilation operators. As an example, for an arbitrary operator $\hat{a}$ acting on a single particle we get

$$\hat{A} = \sum_{pq} \langle p|\hat{a}|q\rangle \, \hat{a}_p^\dagger \hat{a}_q,$$

where, given a single-particle basis $\phi_1, \phi_2 \ldots$, we have the matrix element

$$\langle p|\hat{a}|q\rangle = \int d\mathbf{r} \phi_p^*(\mathbf{r}) \hat{a} \phi_q(\mathbf{r}).$$

The summation indices p and q run over all possible single-particle states. Each operator pair in the sum moves a particle from q to p with probability $\langle p|\hat{a}|q\rangle$, assuming that q is occupied and p is empty.
In the same spirit, an arbitrary two-particle interaction $\hat{B}$ can be written

$$\hat{B} = \frac{1}{4} \sum_{pqrs} \langle pq|\hat{b}|rs\rangle \, \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r.$$

This time the matrix elements are defined as

$$\langle pq|\hat{b}|rs\rangle = \int d\mathbf{r_1} d\mathbf{r_2} \phi_p^*(\mathbf{r_1}) \phi_q^*(\mathbf{r_2}) \hat{b} \phi_r(\mathbf{r_1}) \phi_s(\mathbf{r_2}) - \int d\mathbf{r_1} d\mathbf{r_2} \phi_p^*(\mathbf{r_1}) \phi_q^*(\mathbf{r_2}) \hat{b} \phi_s(\mathbf{r_1}) \phi_r(\mathbf{r_2}),$$

where the second integral provides the antisymmetric property $\langle pq|\hat{b}|rs\rangle = -\langle pq|\hat{b}|sr\rangle$. The factor $\frac{1}{4}$ is needed to account for overcounting:

$$\begin{aligned}
\langle ab|\hat{B}|cd\rangle =& \frac{1}{4} \sum_{pqrs} \langle pq|\hat{b}|rs\rangle \, \langle ab|\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r|cd\rangle \\
=& \frac{1}{4} \Big(\langle ab|\hat{b}|cd\rangle \, \langle ab|\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_d \hat{a}_c|cd\rangle + \langle ba|\hat{b}|cd\rangle \, \langle ab|\hat{a}_b^\dagger \hat{a}_a^\dagger \hat{a}_d \hat{a}_c|cd\rangle \\
& + \langle ab|\hat{b}|dc\rangle \, \langle ab|\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c \hat{a}_d|cd\rangle + \langle ba|\hat{b}|dc\rangle \, \langle ab|\hat{a}_b^\dagger \hat{a}_a^\dagger \hat{a}_c \hat{a}_d|cd\rangle \Big) \\
=& \frac{1}{4} \Big(\langle ab|\hat{b}|cd\rangle - \langle ba|\hat{b}|cd\rangle - \langle ab|\hat{b}|dc\rangle + \langle ba|\hat{b}|dc\rangle \Big) \\
=& \frac{1}{4} 4 \, \langle ab|\hat{b}|cd\rangle = \langle ab|\hat{b}|cd\rangle
\end{aligned}$$

The Hamiltonian (1.2) can now be written as

$$H = \sum_{pq} \langle p|\hat{t}|q\rangle \, \hat{a}_p^\dagger \hat{a}_q + \frac{1}{4} \sum_{pqrs} \langle pq|\hat{v}^{2N}|rs\rangle \, \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r + \frac{1}{36} \sum_{pqrstu} \langle pqr|\hat{v}^{3N}|stu\rangle \, \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r^\dagger \hat{a}_u \hat{a}_t \hat{a}_s.$$

Just as the two-body elements above, the 3N elements $\langle pqr|\hat{v}^{3N}|stu\rangle$ are also antisymmetrised.

2.1.4 Normal-ordered products and contractions

A product of creation and annihilation operators are said to be in *normal order* if all creation operators are to the left of all annihilation operators, e.g.

$$\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r^\dagger \hat{a}_s \hat{a}_t \hat{a}_u$$

is normal-ordered.
A key property of a normal-ordered operator product is that its vacuum expectation value vanishes identically

$$\langle |\, \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r^\dagger \hat{a}_s \hat{a}_t \hat{a}_u \,| \rangle = 0. \tag{2.4}$$

This is obviously true, since the annihilation operators to the right will reduce the empty state to zero before the creation operators can act.
Using the anti-commutation relations (2.1)–(2.3) it is possible to write an arbitrary product of creation and annihilation operators as a sum of normal-ordered products:

$$\begin{aligned}
&\hat{a}_s \hat{a}_r \hat{a}_p^\dagger \hat{a}_q^\dagger = \hat{a}_s \left(\{\hat{a}_r, \hat{a}_p^\dagger\} - \hat{a}_p^\dagger \hat{a}_r \right) \hat{a}_q^\dagger = \delta_{r,p} \hat{a}_s \hat{a}_q^\dagger - \hat{a}_s \hat{a}_p^\dagger \hat{a}_r \hat{a}_q^\dagger \\
&= \delta_{r,p} \left(\{\hat{a}_s, \hat{a}_q^\dagger\} - \hat{a}_q^\dagger \hat{a}_s \right) - \left(\{\hat{a}_s, \hat{a}_p^\dagger\} - \hat{a}_p^\dagger \hat{a}_s \right) \hat{a}_r \hat{a}_q^\dagger \\
&= \delta_{r,p} \delta_{s,q} - \delta_{r,p} \hat{a}_q^\dagger \hat{a}_s - \delta_{s,p} \hat{a}_r \hat{a}_q^\dagger + \hat{a}_p^\dagger \hat{a}_s \hat{a}_r \hat{a}_q^\dagger \\
&= \delta_{r,p} \delta_{s,q} - \delta_{r,p} \hat{a}_q^\dagger \hat{a}_s - \delta_{s,p} \left(\{\hat{a}_r, \hat{a}_q^\dagger\} - \hat{a}_q^\dagger \hat{a}_r \right) + \hat{a}_p^\dagger \hat{a}_s \left(\{\hat{a}_r, \hat{a}_q^\dagger\} - \hat{a}_q^\dagger \hat{a}_r \right) \\
&= \delta_{r,p} \delta_{s,q} - \delta_{r,p} \hat{a}_q^\dagger \hat{a}_s - \delta_{s,p} \delta_{r,q} + \delta_{s,p} \hat{a}_q^\dagger \hat{a}_r + \delta_{r,q} \hat{a}_p^\dagger \hat{a}_s - \hat{a}_p^\dagger \hat{a}_s \hat{a}_q^\dagger \hat{a}_r \\
&= \delta_{r,p} \delta_{s,q} - \delta_{r,p} \hat{a}_q^\dagger \hat{a}_s - \delta_{s,p} \delta_{r,q} + \delta_{s,p} \hat{a}_q^\dagger \hat{a}_r + \delta_{r,q} \hat{a}_p^\dagger \hat{a}_s - \hat{a}_p^\dagger \left(\{\hat{a}_s, \hat{a}_q^\dagger\} - \hat{a}_q^\dagger \hat{a}_s \right) \hat{a}_r \\
&= \delta_{r,p} \delta_{s,q} - \delta_{r,p} \hat{a}_q^\dagger \hat{a}_s - \delta_{s,p} \delta_{q,r} + \delta_{s,p} \hat{a}_q^\dagger \hat{a}_r + \delta_{r,q} \hat{a}_p^\dagger \hat{a}_s - \delta_{s,q} \hat{a}_p^\dagger \hat{a}_r + \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r \\
&= \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r + \delta_{s,p} \hat{a}_q^\dagger \hat{a}_r - \delta_{s,q} \hat{a}_p^\dagger \hat{a}_r - \delta_{r,p} \hat{a}_q^\dagger \hat{a}_s + \delta_{r,q} \hat{a}_p^\dagger \hat{a}_s - \delta_{s,p} \delta_{q,r} + \delta_{r,p} \delta_{s,q}.
\end{aligned} \tag{2.5}$$

The final expression contains five normal-ordered products and two terms without any operators at all. In a similar but even more cumbersome fashion it is possible to normal order longer products. A more convenient method is to use *Wick's theorem* from quantum field theory. Before stating this theorem additional notation must be introduced.
Let $\hat{a}\hat{b}\hat{c}\ldots$ refer to an arbitrary product of creation and annihilation operators. Then the corresponding *normal product* $n[\hat{a}\hat{b}\hat{c}\ldots]$ is a normal-ordered permutation of the original product, with an additional minus sign if the permutation is odd. The normal product can be expressed in several equivalent ways, as illustrated in the following example

$$n[\hat{a}_p^\dagger \hat{a}_r \hat{a}_q^\dagger \hat{a}_s] = -\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s = \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r = -\hat{a}_q^\dagger \hat{a}_p^\dagger \hat{a}_s \hat{a}_r = \hat{a}_q^\dagger \hat{a}_p^\dagger \hat{a}_r \hat{a}_s.$$

Furthermore, the *contraction* of two operators $\hat{a}$ and $\hat{b}$ is defined as

$$\overset{\sqcap}{\hat{a}\hat{b}} = \hat{a}\hat{b} - n[\hat{a}\hat{b}]. \tag{2.6}$$

Operators inside a normal product can be contracted in the following way

$$n[\hat{a}\hat{b}\hat{c}\hat{d}] = -n[\hat{b}\hat{d}\hat{a}\hat{c}] = -\hat{b}\hat{d}n[\hat{a}\hat{c}].$$

In other words, the contracted pair must first be moved in front of the other operators (with a minus sign in the case of odd permutations) before the contraction can be put outside the normal product.

From the anti-commutation relations (2.1)–(2.3) the fermion *contraction rules* can be derived

$$\hat{a}_p\hat{a}_q^\dagger = \hat{a}_p\hat{a}_q^\dagger - n[\hat{a}_p\hat{a}_q^\dagger] = \hat{a}_p\hat{a}_q^\dagger + \hat{a}_q^\dagger\hat{a}_p = \{\hat{a}_p, \hat{a}_q^\dagger\} = \delta_{p,q} \tag{2.7}$$

$$\hat{a}_p^\dagger\hat{a}_q = 0 \tag{2.8}$$

$$\hat{a}_p^\dagger\hat{a}_q^\dagger = 0 \tag{2.9}$$

$$\hat{a}_p\hat{a}_q = 0. \tag{2.10}$$

Note that although the contraction is defined as the difference between two operators products, the end result is an ordinary number.

2.1.5 Wick's theorem

In the context of quantum field theory and many-body physics, Wick's theorem provides a way to turn an arbitrary operator product into a sum of normal-ordered products. The theorem tells us that an operator product is equal to the corresponding normal-ordered product, plus all possible single contractions of the normal-ordered product, plus all possible double contractions of the normal-ordered product, and so on. We can write this as

$$\begin{aligned}\hat{a}\hat{b}\hat{c}\hat{d}\hat{e}\hat{f}\cdots =& n[\hat{a}\hat{b}\hat{c}\hat{d}\hat{e}\hat{f}\ldots] + \sum n[\hat{a}\hat{b}\hat{c}\hat{d}\hat{e}\hat{f}\ldots] \\ &+ \sum n[\hat{a}\hat{b}\hat{c}\hat{d}\hat{e}\hat{f}\ldots] + \sum n[\hat{a}\hat{b}\hat{c}\hat{d}\hat{e}\hat{f}\ldots] + \ldots\end{aligned} \tag{2.11}$$

As an example, consider the operator product from (2.5)

$$\begin{aligned}\hat{a}_s\hat{a}_r\hat{a}_p^\dagger\hat{a}_q^\dagger =& n[\hat{a}_s\hat{a}_r\hat{a}_p^\dagger\hat{a}_q^\dagger] + n[\hat{a}_s\hat{a}_r\hat{a}_p^\dagger\hat{a}_q^\dagger] + n[\hat{a}_s\hat{a}_r\hat{a}_p^\dagger\hat{a}_q^\dagger] + n[\hat{a}_s\hat{a}_r\hat{a}_p^\dagger\hat{a}_q^\dagger] \\ &+ n[\hat{a}_s\hat{a}_r\hat{a}_p^\dagger\hat{a}_q^\dagger] + n[\hat{a}_s\hat{a}_r\hat{a}_p^\dagger\hat{a}_q^\dagger] + n[\hat{a}_s\hat{a}_r\hat{a}_p^\dagger\hat{a}_q^\dagger] \\ =& n[\hat{a}_s\hat{a}_r\hat{a}_p^\dagger\hat{a}_q^\dagger] - \hat{a}_s\hat{a}_p^\dagger n[\hat{a}_r\hat{a}_q^\dagger] + \hat{a}_s\hat{a}_q^\dagger n[\hat{a}_r\hat{a}_p^\dagger] + \hat{a}_r\hat{a}_p^\dagger n[\hat{a}_s\hat{a}_q^\dagger] \\ &- \hat{a}_r\hat{a}_q^\dagger n[\hat{a}_s\hat{a}_p^\dagger] - \hat{a}_s\hat{a}_p^\dagger\hat{a}_r\hat{a}_q^\dagger + \hat{a}_s\hat{a}_q^\dagger\hat{a}_r\hat{a}_p^\dagger \\ =& \hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_s\hat{a}_r + \delta_{s,p}\hat{a}_q^\dagger\hat{a}_r - \delta_{s,q}\hat{a}_p^\dagger\hat{a}_r - \delta_{r,p}\hat{a}_q^\dagger\hat{a}_s \\ &+ \delta_{r,q}\hat{a}_p^\dagger\hat{a}_s - \delta_{s,p}\delta_{r,q} + \delta_{s,q}\delta_{r,p}\end{aligned} \tag{2.12}$$

The contraction rule (2.7) has been used above. Contractions corresponding to (2.8)–(2.10) are trivially zero and have been omitted. Note that we have arrived at the same result as in (2.5) but with less work.

2.1.6 Normal-ordering and Fermi states

We have previously demonstrated how an arbitrary many-body state can be constructed by applying a series of creation operators to the vacuum $|\rangle$. It is also possible to use a non-empty Fermi state $|\Phi\rangle$ as a starting point. We refer to $|\Phi\rangle$ as

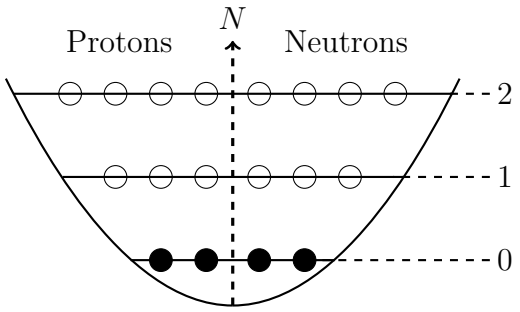


Figure 2.1: The Fermi state of Helium-4 with hole states represented as filled circles and particle states as unfilled circles. Note that the $N = 1$ and $N = 2$ shells contain more single-particle states than indicated.

a *reference state* or a *Fermi vacuum*. Single-particle states that are occupied in $|\Phi\rangle$ are called *hole states*, whereas unoccupied states are called *particle states*. This is illustrated in Figure 2.1. A common notation is to use the letters $i, j, k \dots$ to denote hole states, $a, b, c \dots$ for particle states and $p, q, r \dots$ for arbitrary single-particle states.

Given a certain reference state $|\Phi\rangle$, creation operators $\hat{a}_a^\dagger$ acting on particle states and annihilation operators $\hat{a}_i$ acting on hole states are considered *pseudo-creation operators*. Similarly, annihilation operators $\hat{a}_a$ acting on particle states and creation operators $\hat{a}_i^\dagger$ acting on hole states are known as *pseudo-annihilation operators*. A pseudo-annihilation operator applied to $|\Phi\rangle$ will result in zero, as this implies either trying to annihilate an unoccupied particle state or trying to populate an already occupied hole state. This is completely analogous to the way ordinary annihilation operators turn the vacuum ket $|\rangle$ into zero.

The concept of normal ordering can now be extended in the following way: An operator product is said to be in normal order *with respect to* a reference state $|\Phi\rangle$ if all pseudo-creation operators are to the left of all pseudo-annihilation operators. The ordinary normal order introduced before is also known as *vacuum normal order*. Although one can define normal order relative to several reference states, this thesis will only deal with *single-reference* normal ordering.

Analogously to the ordinary normal product $n[\hat{a}\hat{b}\hat{c}\dots]$ we define $\{\hat{a}\hat{b}\hat{c}\dots\}$ as the normal product of $\hat{a}\hat{b}\hat{c}\dots$ with respect to $|\Phi\rangle$. Note that the reference state expectation value of such a product is identically zero

$$\langle\Phi|\{\hat{a}\hat{b}\hat{c}\dots\}_{|\Phi\rangle}|\Phi\rangle = 0 \tag{2.13}$$

since any pseudo-annihilation operators will be moved to the right and turn $|\Phi\rangle$ into zero and any pseudo-creation operator will be moved to the left and turn $\langle\Phi|$ into zero. This property mirrors (2.4) and is the motivation for defining reference normal ordering as above.

With the normal product definition above, the corresponding contraction can be defined as

$$\hat{a}\hat{b} = \hat{a}\hat{b} - \{\hat{a}\hat{b}\}. \tag{2.14}$$

It can be shown that this contraction only results in non-zero values in the following

two cases

$$\hat{a}_a \overbrace{\hat{a}_b^\dagger} = \delta_{a,b}$$
$$\hat{a}_i^\dagger \overbrace{\hat{a}_j} = \delta_{i,j}.$$

We can express the above as

$$\hat{a}_p \overbrace{\hat{a}_q^\dagger} = \delta_{p,q>F} \tag{2.15}$$
$$\hat{a}_p^\dagger \overbrace{\hat{a}_q} = \delta_{p,q<F} \tag{2.16}$$

where $\delta_{p,q>F}$ confines p and q to particle states (above the Fermi level F) and $\delta_{p,q<F}$ confines p and q to hole states (below the Fermi level F).
Wick's theorem is also valid in the context of normal ordering with respect to a reference state. In this case (2.11) turns into

$$\begin{aligned}\hat{a}\hat{b}\hat{c}\hat{d}\hat{e}\hat{f}\cdots = &\{\hat{a}\hat{b}\hat{c}\hat{d}\hat{e}\hat{f}\ldots\} + \sum\{\hat{a}\overbrace{\hat{b}\hat{c}}\hat{d}\hat{e}\hat{f}\ldots\} \\ &+ \sum\{\hat{a}\overbrace{\hat{b}\hat{c}}\overbrace{\hat{d}\hat{e}}\hat{f}\ldots\} + \sum\{\hat{a}\overbrace{\hat{b}\hat{c}}\overbrace{\hat{d}\hat{e}}\overbrace{\hat{f}}\} + \ldots\end{aligned} \tag{2.17}$$

2.2 Normal-ordered approximations

2.2.1 Derivation

The starting point of the NO2B approximation is the 3N interaction in vacuum normal order

$$\hat{V}^{3N} = \frac{1}{36}\sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\, \hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s. \tag{2.18}$$

Using Wick's theorem (2.17) this can be rewritten as sum of operators normal-ordered with respect to the Fermi state of the nucleus in interest.

$$\begin{aligned}\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s = &\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \sum\{\hat{a}_p^\dagger\overbrace{\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u}\hat{a}_t\hat{a}_s\} \\ &+ \sum\{\overbrace{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u}\hat{a}_t\hat{a}_s\} + \sum\{\overbrace{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s}\}.\end{aligned} \tag{2.19}$$

In the above expression the three sums are taken over all single contractions, all double contractions and all triple contractions, respectively.
Due to the number of terms involved it is convenient to expand each sum separately. Using the contraction rule (2.16) the single contractions can be rewritten in the

following way

$$\begin{aligned}
\sum\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} &= \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
&+ \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
&+ \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
&= \delta_{p,u<F}\{\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_t\hat{a}_s\} - \delta_{p,t<F}\{\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_s\} + \delta_{p,s<F}\{\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\} \\
&- \delta_{q,u<F}\{\hat{a}_p^\dagger\hat{a}_r^\dagger\hat{a}_t\hat{a}_s\} + \delta_{q,t<F}\{\hat{a}_p^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_s\} - \delta_{q,s<F}\{\hat{a}_p^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\} \\
&+ \delta_{r,u<F}\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\} - \delta_{r,t<F}\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_u\hat{a}_s\} + \delta_{r,s<F}\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_u\hat{a}_t\}.
\end{aligned}$$

Note the sign changes emerging when moving the contracted operators to the beginning of the operator products.
We now add the summation over p, q, r, s, t and u. In each term the delta function combines two of the summation indices into a single index i, which is restricted to the hole states (i.e. the single-particle states occupied in $|\Phi\rangle$). By rearranging the indices inside the matrix element (and switching signs in the case of odd permutations) we see that all 9 terms are in fact identical.

$$\begin{aligned}
&\sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\sum\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
&= \sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\,\delta_{p,u<F}\{\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_t\hat{a}_s\} - \sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\,\delta_{p,t<F}\{\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_s\} \\
&+ \sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\,\delta_{p,s<F}\{\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\} - \sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\,\delta_{q,u<F}\{\hat{a}_p^\dagger\hat{a}_r^\dagger\hat{a}_t\hat{a}_s\} \\
&+ \sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\,\delta_{q,t<F}\{\hat{a}_p^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_s\} - \sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\,\delta_{q,s<F}\{\hat{a}_p^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\} \\
&+ \sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\,\delta_{r,u<F}\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\} - \sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\,\delta_{r,t<F}\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_u\hat{a}_s\} \\
&+ \sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\,\delta_{r,s<F}\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_u\hat{a}_t\} \\
&= \sum_{iqrst}\langle iqr|\hat{v}^{3N}|sti\rangle\,\{\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_t\hat{a}_s\} - \sum_{iqrsu}\langle iqr|\hat{v}^{3N}|siu\rangle\,\{\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_s\} \\
&+ \sum_{iqrtu}\langle iqr|\hat{v}^{3N}|itu\rangle\,\{\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\} - \sum_{iprst}\langle pir|\hat{v}^{3N}|sti\rangle\,\{\hat{a}_p^\dagger\hat{a}_r^\dagger\hat{a}_t\hat{a}_s\} \\
&+ \sum_{iprsu}\langle pir|\hat{v}^{3N}|siu\rangle\,\{\hat{a}_p^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_s\} - \sum_{iprtu}\langle pir|\hat{v}^{3N}|itu\rangle\,\{\hat{a}_p^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\} \\
&+ \sum_{ipqst}\langle pqi|\hat{v}^{3N}|sti\rangle\,\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\} - \sum_{ipqsu}\langle pqi|\hat{v}^{3N}|siu\rangle\,\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_u\hat{a}_s\} \\
&+ \sum_{ipqtu}\langle pqi|\hat{v}^{3N}|itu\rangle\,\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_u\hat{a}_t\} \\
&= 9\sum_{ipqst}\langle pqi|\hat{v}^{3N}|sti\rangle\,\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\}
\end{aligned}$$

The sum over all double contractions is slightly more intricate but follows the same principle.

$$
\begin{aligned}
\sum\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} = {} & \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
& + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
& + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
& + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
& + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
& + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
& = \\
& - \delta_{p,u<F}\delta_{q,t<F}\{\hat{a}_r^\dagger\hat{a}_s\} + \delta_{p,u<F}\delta_{q,s<F}\{\hat{a}_r^\dagger\hat{a}_t\} + \delta_{p,t<F}\delta_{q,u<F}\{\hat{a}_r^\dagger\hat{a}_s\} \\
& - \delta_{p,t<F}\delta_{q,s<F}\{\hat{a}_r^\dagger\hat{a}_u\} - \delta_{p,s<F}\delta_{q,u<F}\{\hat{a}_r^\dagger\hat{a}_t\} + \delta_{p,s<F}\delta_{q,t<F}\{\hat{a}_r^\dagger\hat{a}_u\} \\
& + \delta_{p,u<F}\delta_{r,t<F}\{\hat{a}_q^\dagger\hat{a}_s\} - \delta_{p,u<F}\delta_{r,s<F}\{\hat{a}_q^\dagger\hat{a}_t\} - \delta_{p,t<F}\delta_{r,u<F}\{\hat{a}_q^\dagger\hat{a}_s\} \\
& + \delta_{p,t<F}\delta_{r,s<F}\{\hat{a}_q^\dagger\hat{a}_u\} + \delta_{p,s<F}\delta_{r,u<F}\{\hat{a}_q^\dagger\hat{a}_t\} - \delta_{p,s<F}\delta_{r,t<F}\{\hat{a}_q^\dagger\hat{a}_u\} \\
& - \delta_{q,u<F}\delta_{r,t<F}\{\hat{a}_p^\dagger\hat{a}_s\} + \delta_{q,u<F}\delta_{r,s<F}\{\hat{a}_p^\dagger\hat{a}_t\} + \delta_{q,t<F}\delta_{r,u<F}\{\hat{a}_p^\dagger\hat{a}_s\} \\
& - \delta_{q,t<F}\delta_{r,s<F}\{\hat{a}_p^\dagger\hat{a}_u\} - \delta_{q,s<F}\delta_{r,u<F}\{\hat{a}_p^\dagger\hat{a}_t\} + \delta_{q,s<F}\delta_{r,t<F}\{\hat{a}_p^\dagger\hat{a}_u\}
\end{aligned}
$$

Since each term contains two delta functions four of the summation indices p, q, r, s, t, u are fused into two hole indices i and j, only leaving a single pair as free indices.

As before, all terms are identical.

$$
\begin{aligned}
&\sum_{pqrstu} \langle pqr|\hat{v}^{3N}|stu\rangle \sum\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} = \\
&-\sum_{ijrs} \langle ijr|\hat{v}^{3N}|sji\rangle \{\hat{a}_r^\dagger\hat{a}_s\} + \sum_{ijrt} \langle ijr|\hat{v}^{3N}|jti\rangle \{\hat{a}_r^\dagger\hat{a}_t\} \\
&+\sum_{ijrs} \langle ijr|\hat{v}^{3N}|sij\rangle \{\hat{a}_r^\dagger\hat{a}_s\} - \sum_{ijru} \langle ijr|\hat{v}^{3N}|jiu\rangle \{\hat{a}_r^\dagger\hat{a}_u\} \\
&-\sum_{ijrt} \langle ijr|\hat{v}^{3N}|itj\rangle \{\hat{a}_r^\dagger\hat{a}_t\} + \sum_{ijru} \langle ijr|\hat{v}^{3N}|iju\rangle \{\hat{a}_r^\dagger\hat{a}_u\} \\
&+\sum_{ijqs} \langle iqj|\hat{v}^{3N}|sji\rangle \{\hat{a}_q^\dagger\hat{a}_s\} - \sum_{ijqt} \langle iqj|\hat{v}^{3N}|jti\rangle \{\hat{a}_q^\dagger\hat{a}_t\} \\
&-\sum_{ijqs} \langle iqj|\hat{v}^{3N}|sij\rangle \{\hat{a}_q^\dagger\hat{a}_s\} + \sum_{ijqu} \langle iqj|\hat{v}^{3N}|jiu\rangle \{\hat{a}_q^\dagger\hat{a}_u\} \\
&+\sum_{ijqt} \langle iqj|\hat{v}^{3N}|itj\rangle \{\hat{a}_q^\dagger\hat{a}_t\} - \sum_{ijqu} \langle iqj|\hat{v}^{3N}|iju\rangle \{\hat{a}_q^\dagger\hat{a}_u\} \\
&-\sum_{ijps} \langle pij|\hat{v}^{3N}|sji\rangle \{\hat{a}_p^\dagger\hat{a}_s\} + \sum_{ijpt} \langle pij|\hat{v}^{3N}|jti\rangle \{\hat{a}_p^\dagger\hat{a}_t\} \\
&+\sum_{ijps} \langle pij|\hat{v}^{3N}|sij\rangle \{\hat{a}_p^\dagger\hat{a}_s\} - \sum_{ijpu} \langle pij|\hat{v}^{3N}|jiu\rangle \{\hat{a}_p^\dagger\hat{a}_u\} \\
&-\sum_{ijpt} \langle pij|\hat{v}^{3N}|jti\rangle \{\hat{a}_p^\dagger\hat{a}_t\} + \sum_{ijpu} \langle pij|\hat{v}^{3N}|iju\rangle \{\hat{a}_p^\dagger\hat{a}_u\} \\
&= 18 \sum_{ijps} \langle pij|\hat{v}^{3N}|sij\rangle \{\hat{a}_p^\dagger\hat{a}_s\}
\end{aligned}
$$

Finally, the sum over all triple contractions only yields six terms.

$$
\begin{aligned}
\sum\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} &= \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
&+ \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} + \{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} \\
&= \\
&- \delta_{p,u<F}\delta_{q,t<F}\delta_{r,s<F} + \delta_{p,u<F}\delta_{q,s<F}\delta_{r,t<F} + \delta_{p,t<F}\delta_{q,u<F}\delta_{r,s<F} \\
&- \delta_{p,t<F}\delta_{q,s<F}\delta_{r,u<F} - \delta_{p,s<F}\delta_{q,u<F}\delta_{r,t<F} + \delta_{p,s<F}\delta_{q,t<F}\delta_{r,u<F}
\end{aligned}
$$

The three delta functions in each term combine the six summation indices into three hole indices ijk. As all operators are contracted this leaves us with a sum of six identical constant terms.

$$
\begin{aligned}
&\sum_{pqrstu} \langle pqr|\hat{v}^{3N}|stu\rangle \sum\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\} = \\
&-\sum_{ijk} \langle ijk|\hat{v}^{3N}|kji\rangle + \sum_{ijk} \langle ijk|\hat{v}^{3N}|jki\rangle + \sum_{ijk} \langle ijk|\hat{v}^{3N}|kij\rangle \\
&-\sum_{ijk} \langle ijk|\hat{v}^{3N}|jik\rangle - \sum_{ijk} \langle ijk|\hat{v}^{3N}|ikj\rangle + \sum_{ijk} \langle ijk|\hat{v}^{3N}|ijk\rangle \\
&= 6 \sum_{ijk} \langle ijk|\hat{v}^{3N}|ijk\rangle
\end{aligned}
$$

The result of the three contraction sums above can be inserted into (2.18) yielding

$$\begin{aligned}\hat{V}^{3N} = &\frac{1}{36}\sum_{pqrstu}\langle pqr|\hat{v}^{3N}|stu\rangle\,\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_r^\dagger\hat{a}_u\hat{a}_t\hat{a}_s\}\\ &+\frac{1}{4}\sum_{ipqst}\langle pqi|\hat{v}^{3N}|sti\rangle\,\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\}+\frac{1}{2}\sum_{ijps}\langle pij|\hat{v}^{3N}|sij\rangle\,\{\hat{a}_p^\dagger\hat{a}_s\}+\frac{1}{6}\sum_{ijk}\langle ijk|\hat{v}^{3N}|ijk\rangle\,.\end{aligned}$$

The interpretation of these four terms has already been presented in the introduction — the 0N, 1N, 2N, and 3N terms then correspond to transitions with three, two, one and zero diagonal single-particle states that belong to the Fermi configuration. If we remove the three-body term from the expression above we arrive at the normal-ordered two-body (NO2B) approximation

$$\begin{aligned}\hat{V}^{NO2B} =&\frac{1}{4}\sum_{ipqst}\langle pqi|\hat{v}^{3N}|sti\rangle\,\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\}+\frac{1}{2}\sum_{ijps}\langle pij|\hat{v}^{3N}|sij\rangle\,\{\hat{a}_p^\dagger\hat{a}_s\}\\ &+\frac{1}{6}\sum_{ijk}\langle ijk|\hat{v}^{3N}|ijk\rangle\,.\end{aligned}\tag{2.20}$$

Analogously we also get the normal-ordered one-body (NO1B) approximation

$$\hat{V}^{NO1B} = \frac{1}{2}\sum_{ijps}\langle pij|\hat{v}^{3N}|sij\rangle\,\{\hat{a}_p^\dagger\hat{a}_s\}+\frac{1}{6}\sum_{ijk}\langle ijk|\hat{v}^{3N}|ijk\rangle\tag{2.21}$$

and the normal-ordered zero-body (NO0B) approximation

$$\hat{V}^{NO0B} = \frac{1}{6}\sum_{ijk}\langle ijk|\hat{v}^{3N}|ijk\rangle\,.\tag{2.22}$$

2.2.2 Returning to vacuum normal order

Before (2.20) can be used in the no-core shell model it must be converted back into vacuum normal order. This can be done by using Wick's theorem in reverse. In the one-body case

$$\hat{a}_p^\dagger\hat{a}_s = \{\hat{a}_p^\dagger\hat{a}_s\} + \hat{a}_p^\dagger\hat{a}_s = \{\hat{a}_p^\dagger\hat{a}_s\} + \delta_{p,s<F}$$

this is trivial, as we only have to move the delta function to the opposite side of the equation

$$\{\hat{a}_p^\dagger\hat{a}_s\} = \hat{a}_p^\dagger\hat{a}_s - \hat{a}_p^\dagger\hat{a}_s = \{\hat{a}_p^\dagger\hat{a}_s\} - \delta_{p,s<F}.\tag{2.23}$$

In the 2B-case we apply the same principle, and use (2.23) to invert the resulting

one-body terms

$$\begin{aligned}
\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s =&\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\} + \{\overbrace{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t}\hat{a}_s\} + \{\overbrace{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s}\} + \{\hat{a}_p^\dagger\overbrace{\hat{a}_q^\dagger\hat{a}_t}\hat{a}_s\} \\
&+ \{\overbrace{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t}\hat{a}_s\} + \{\hat{a}_p^\dagger\overbrace{\hat{a}_q^\dagger\hat{a}_t\hat{a}_s}\} + \{\hat{a}_p^\dagger\overbrace{\hat{a}_q^\dagger\hat{a}_t}\hat{a}_s\} \\
=&\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\} - \delta_{p,t<F}\{\hat{a}_q^\dagger\hat{a}_s\} + \delta_{p,s<F}\{\hat{a}_q^\dagger\hat{a}_t\} + \delta_{q,t<F}\{\hat{a}_p^\dagger\hat{a}_s\} \\
&- \delta_{q,s<F}\{\hat{a}_p^\dagger\hat{a}_t\} - \delta_{p,t<F}\delta_{q,s<F} + \delta_{p,s<F}\delta_{q,t<F} \\
=&\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\} - \delta_{p,t<F}(\hat{a}_q^\dagger\hat{a}_s - \delta_{q,s<F}) + \delta_{p,s<F}(\hat{a}_q^\dagger\hat{a}_t - \delta_{q,t<F}) + \delta_{q,t<F}(\hat{a}_p^\dagger\hat{a}_s - \delta_{p,s<F}) \\
&- \delta_{q,s<F}(\hat{a}_p^\dagger\hat{a}_t - \delta_{p,tt<F}) - \delta_{p,t<F}\delta_{q,s<F} + \delta_{p,s<F}\delta_{q,t<F} \\
=&\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\} - \delta_{p,t<F}\hat{a}_q^\dagger\hat{a}_s + \delta_{p,s<F}\hat{a}_q^\dagger\hat{a}_t + \delta_{q,t<F}\hat{a}_p^\dagger\hat{a}_s \\
&- \delta_{q,s<F}\hat{a}_p^\dagger\hat{a}_t + \delta_{p,t<F}\delta_{q,s<F} - \delta_{p,s<F}\delta_{q,t<F}
\end{aligned} .$$

As before we simply move all terms containing delta functions to the opposite side of the equation, resulting in

$$\begin{aligned}
\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\} =&\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s + \delta_{p,t<F}\hat{a}_q^\dagger\hat{a}_s - \delta_{p,s<F}\hat{a}_q^\dagger\hat{a}_t - \delta_{q,t<F}\hat{a}_p^\dagger\hat{a}_s \\
&+ \delta_{q,s<F}\hat{a}_p^\dagger\hat{a}_t - \delta_{p,t<F}\delta_{q,s<F} + \delta_{p,s<F}\delta_{q,t<F}.
\end{aligned} \tag{2.24}$$

Inserting (2.23) into the the one-body term of (2.20) gives us

$$\begin{aligned}
\sum_{ijps}\langle pij|\hat{v}^{3N}|sij\rangle\,\{\hat{a}_p^\dagger\hat{a}_s\} &= \sum_{ijps}\langle pij|\hat{v}^{3N}|sij\rangle\,\hat{a}_p^\dagger\hat{a}_s - \sum_{ijps}\langle pij|\hat{v}^{3N}|sij\rangle\,\delta_{p,s<F} \\
&= \sum_{ijps}\langle pij|\hat{v}^{3N}|sij\rangle\,\hat{a}_p^\dagger\hat{a}_s - \sum_{ijk}\langle ijk|\hat{v}^{3N}|ijk\rangle\,.
\end{aligned}$$

Similarly, inserting (2.24) into the two-body term of (2.20) produces

$$\begin{aligned}
&\sum_{ipqst}\langle pqi|\hat{v}^{3N}|sti\rangle\,\{\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s\} = \sum_{ipqst}\langle pqi|\hat{v}^{3N}|sti\rangle\,\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s \\
&+\sum_{ijqs}\langle jqi|\hat{v}^{3N}|sji\rangle\,\hat{a}_q^\dagger\hat{a}_s - \sum_{ijqt}\langle jqi|\hat{v}^{3N}|jti\rangle\,\hat{a}_q^\dagger\hat{a}_t - \sum_{ijps}\langle pji|\hat{v}^{3N}|sji\rangle\,\hat{a}_p^\dagger\hat{a}_s \\
&+\sum_{ijpt}\langle pji|\hat{v}^{3N}|jti\rangle\,\hat{a}_p^\dagger\hat{a}_t - \sum_{ijk}\langle jki|\hat{v}^{3N}|kji\rangle + \sum_{ijk}\langle jki|\hat{v}^{3N}|jki\rangle \\
&= \sum_{ipqst}\langle pqi|\hat{v}^{3N}|sti\rangle\,\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s - 4\sum_{ijps}\langle pij|\hat{v}^{3N}|sij\rangle\,\hat{a}_p^\dagger\hat{a}_s + 2\sum_{ijk}\langle ijk|\hat{v}^{3N}|ijk\rangle\,.
\end{aligned}$$

The rewritten terms above transform (2.20) into vacuum normal order

$$\begin{aligned}
\hat{V}^{NO2B} =&\frac{1}{4}\left(\sum_{ipqst}\langle pqi|\hat{v}^{3N}|sti\rangle\,\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s - 4\sum_{ijps}\langle pij|\hat{v}^{3N}|sij\rangle\,\hat{a}_p^\dagger\hat{a}_s + 2\sum_{ijk}\langle ijk|\hat{v}^{3N}|ijk\rangle\right) \\
&+\frac{1}{2}\left(\sum_{ijps}\langle pij|\hat{v}^{3N}|sij\rangle\,\hat{a}_p^\dagger\hat{a}_s - \sum_{ijk}\langle ijk|\hat{v}^{3N}|ijk\rangle\right) + \frac{1}{6}\sum_{ijk}\langle ijk|\hat{v}^{3N}|ijk\rangle \\
=&\frac{1}{4}\sum_{ipqst}\langle pqi|\hat{v}^{3N}|sti\rangle\,\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s - \frac{1}{2}\sum_{ijps}\langle pij|\hat{v}^{3N}|sij\rangle\,\hat{a}_p^\dagger\hat{a}_s + \frac{1}{6}\sum_{ijk}\langle ijk|\hat{v}^{3N}|ijk\rangle\,.
\end{aligned}$$

This can be expressed more succinctly as

$$\hat{V}^{NO2B} = \frac{1}{4}\sum_{pqst} v_{pqst}\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_t\hat{a}_s - \frac{1}{2}\sum_{ps} v_{ps}\hat{a}_p^\dagger\hat{a}_s + v, \tag{2.25}$$

where

$$v_{pqst} = \sum_i \langle pqi|\hat{v}^{3N}|sti\rangle \tag{2.26}$$

$$v_{ps} = \sum_{ij} \langle pij|\hat{v}^{3N}|sij\rangle \tag{2.27}$$

$$v = \frac{1}{6}\sum_{ijk} \langle ijk|\hat{v}^{3N}|ijk\rangle\,. \tag{2.28}$$

Using the notation above, the NO1B approximation (2.21) in vacuum normal order is

$$\hat{V}^{NO1B} = \frac{1}{2}\sum_{ps} v_{ps}\hat{a}_p^\dagger\hat{a}_s - 2v. \tag{2.29}$$

The NO0B approximation (2.22) only contains a constant term and is thus the same in vacuum normal order

$$\hat{V}^{NO0B} = v. \tag{2.30}$$

2.2.3 Expressing lower-order operators as 2N operators

A complication inherent to the NO2B approximation is the appearance of the one-body and constant terms, in addition to the usual two-body term. By expressing the two former as two-body operators this problem can be circumvented without having to rewrite other software packages to accommodate the additional terms.
As a starting point consider the number operator

$$\hat{N} = \sum_p \hat{a}_p^\dagger\hat{a}_p,$$

which returns the number of particles in a many-body state.
Since for any N-body state $|a_1a_2\ldots a_N\rangle$

$$\langle a_1a_2\ldots a_N|\hat{N}|a_1a_2\ldots a_N\rangle = N$$

it is obvious that we can construct a one-body identity operator as

$$\hat{1}_1 = \frac{1}{N}\hat{N} = \frac{1}{N}\sum_p \hat{a}_p^\dagger\hat{a}_p.$$

To arrive at a two-body identity operator we start from a similar expression

$$\hat{N}^2 = \sum_{pq} \hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_q\hat{a}_p,$$

which has the following effect

$$\langle a_1a_2\ldots a_N|\hat{N}^2|a_1a_2\ldots a_N\rangle = \langle a_1a_2\ldots a_N|\sum_p \hat{a}_p^\dagger\left(\sum_q \hat{a}_q^\dagger\hat{a}_q\right)\hat{a}_p|a_1a_2\ldots a_N\rangle = N(N-1).$$

Since the inner operator pair $\sum_q \hat{a}_q^\dagger \hat{a}_q$ will act on a ket which has already been reduced by one particle by the rightmost annihilation operator $\hat{a}_p$, the result is $N(N-1)$ rather than N^2. This gives us the identity operator

$$\hat{1}_2 = \frac{1}{N(N-1)}\hat{N^2} = \frac{1}{N(N-1)}\sum_{pq}\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_q \hat{a}_p.$$

We now utilise the identity operator above to write the constant term as a two-body interaction

$$v = \hat{1}_2 v = \frac{1}{N(N-1)} v\hat{N^2} = \frac{1}{N(N-1)}\sum_{pq} v\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_q \hat{a}_p.$$

This is not yet in the same form as the 2N term in (2.25), as we only have two summation indices. We can add two more in the following fashion:

$$\begin{aligned} v &= \frac{1}{N(N-1)}\sum_{pq} v\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_q \hat{a}_p = \frac{1}{N(N-1)}\sum_{pqst} v\frac{\delta_{p,s}\delta_{q,t} - \delta_{p,t}\delta_{q,s}}{2}\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_t \hat{a}_s \\ &= \frac{1}{4}\sum_{pqst}\frac{2v}{N(N-1)}\left(\delta_{p,s}\delta_{q,t} - \delta_{p,t}\delta_{q,s}\right)\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_t \hat{a}_s \end{aligned} \tag{2.31}$$

The one-body term can be rewritten in the same way:

$$\begin{aligned} \sum_{ps} v_{ps}\hat{a}_p^\dagger \hat{a}_s &= \sum_{ps} v_{ps}\hat{a}_p^\dagger \frac{1}{N-1}\hat{N}\hat{a}_s = \frac{1}{N-1}\sum_{pqs} v_{ps}\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_q \hat{a}_s \\ &= \frac{1}{N-1}\sum_{pqst}(v_{ps}\delta_{q,t} - v_{pt}\delta_{q,s} - v_{qs}\delta_{p,t} + v_{qt}\delta_{p,s})\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_t \hat{a}_s. \end{aligned} \tag{2.32}$$

Just as before the $\hat{N}$ is divided by $N-1$ and not N since $\hat{a}_s$ removes one particle from the ket before $\hat{N}$ can act.

2.3 Coupled and uncoupled matrix elements

Many-body states can be expressed in terms of uncoupled single-particle states. Consider the two-body case

$$|ab\rangle = |n_a, l_a, s_a, j_a, m_a, t_a, t_{za}; n_b, l_b, s_b, j_b, m_b, t_b, t_{zb}\rangle\,.$$

This is known as the m-scheme representation. In this thesis the single-particle states are expressed in a harmonic-oscillator basis. Above, n and l are the quantum numbers for the oscillator whereas s is the particle spin. Furthermore, j refers to the total angular momentum and t refers to the isospin of the particle. m and t_z, respectively, are the corresponding projection quantum numbers. Since $s = \frac{1}{2}$ and $t = \frac{1}{2}$ for all nucleons they are often omitted.
It should be noted that the labels a, b, c and d used in this context refer to arbitrary single-particle states, and are not related to the notation introduced in 2.1.6 (where they were used to indicate particle states).

An alternative to the m-scheme representation is to use spin-coupled states. Spin-coupling can be performed in both spin and isospin space by coupling j_a and j_b to a total angular momentum J and by coupling t_a and t_b to a total isospin T. Coupling both sets of spin is known as JT-coupling. An advantage of this over the m-scheme is that interactions can be represented using fewer matrix elements, reducing the amount of storage required.
It can be shown [15] that the following relation holds between coupled and uncoupled two-body matrix elements

$$\begin{aligned}
&\langle ab; JT|V|cd; JT\rangle \\
&= \langle (n_a, l_a, j_a), (n_b, l_b, j_b); JT|V|(n_c, l_c, j_c), (n_d, l_d, j_d); JT\rangle \\
&= N_{ab}(JT)N_{cd}(JT) \sum_{m_a,m_b,m_c,m_d} \langle j_a m_a j_b m_b|JM\rangle \langle j_c m_c j_d m_d|JM\rangle \\
&\times \sum_{t_{za},t_{zb},t_{zc},t_{zd}} \left\langle \frac{1}{2} t_{za} \frac{1}{2} t_{zb} \middle| TM_T \right\rangle \left\langle \frac{1}{2} t_{zc} \frac{1}{2} t_{zd} \middle| TM_T \right\rangle \\
&\times \langle n_a, l_a, j_a, m_a, t_{za}, n_b, l_b, j_b, m_b, t_{zb}|V|n_c, l_c, j_c, m_c, t_{zc}, n_d, l_d, j_d, m_d, t_{zd}\rangle
\end{aligned} \quad . \tag{2.33}$$

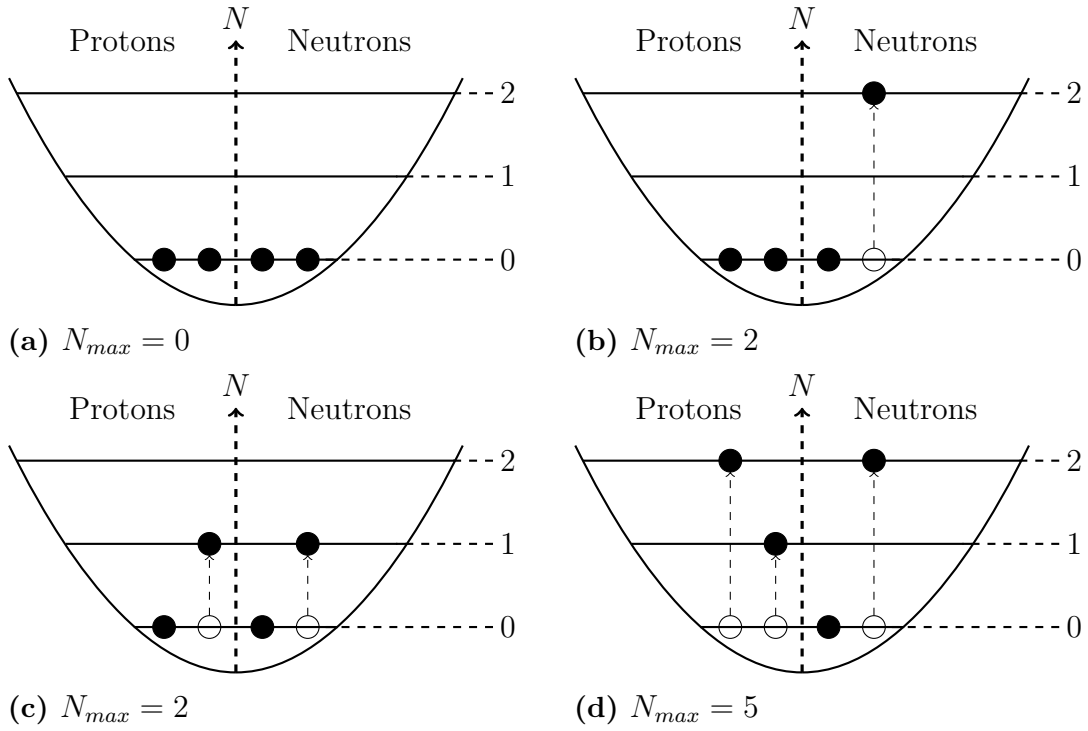
The terms following the summation symbols are Clebsch-Gordan coefficients, whereas the two prefactors are normalisation coefficients defined as

$$N_{ab}(JT) = \frac{\sqrt{1 - \delta_{ab}(-1)^{J+T}}}{1 + \delta_{ab}}.$$

Note that J and T are conserved by all interactions without isospin-breaking terms.

2.4 Model space truncation

As mentioned in the introduction, the Schrödinger equation is turned into a finite matrix equation by expressing the Hamiltonian in a truncated basis. This sets an upper limit to our model space. In this thesis the truncation is controlled by the N_{max} parameter, which denotes the maximum number of harmonic oscillator excitations above the Fermi state. For example, if $N_{max} = 2$ only states that can be reached from the Fermi state with two or less excitations are included. N_{max} for various many-body configurations of helium-4 is shown in Figure 2.2. The size of the model space (i.e. the number of many-body basis states) increases dramatically as N_{max} grows.



(a) $N_{max} = 0$ **(b)** $N_{max} = 2$

(c) $N_{max} = 2$ **(d)** $N_{max} = 5$

Figure 2.2: The value of N_{max} for various many-body configurations of helium-4.

3
Implementation

To test the concepts presented in the preceding chapter a simple implementation named `pyNO2B` was written in the Python programming language. Given two files containing two-nucleon (2N) and three-nucleon (3N) matrix elements, respectively, it computes the approximated NO2B matrix elements from the 3N interaction and adds them to the 2N matrix elements. The resulting 2N+3N(NO2B) matrix elements are then written to a file which can be used as an input to many-body calculations.

3.1 Overview

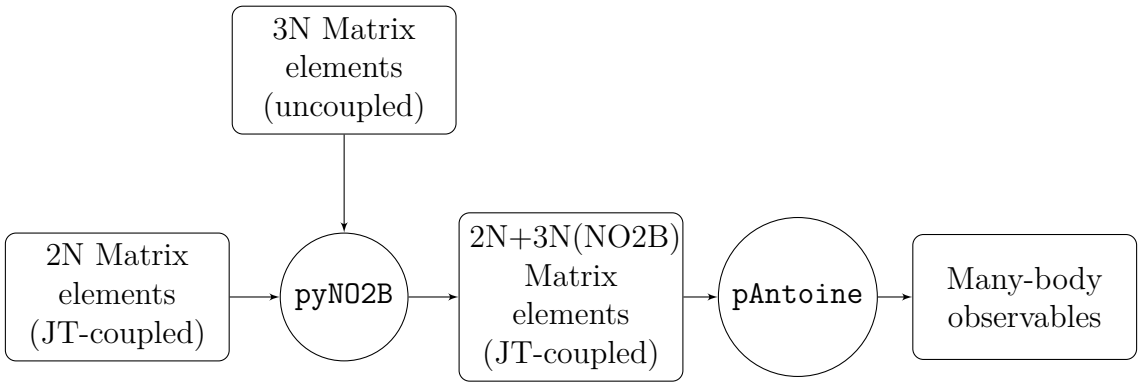


Figure 3.1: Computing NO2B-approximated observables from 2N and 3N interactions using the `pyNO2B` code and the `pAntoine` many-body solver.

The usage of `pyNO2B` is illustrated in Figure 3.1. The resulting output is fed to `pAntoine`, a many-body code based on the No-Core Shell Model [1, 3]. Although several different many-body observables can be calculated, only ground-state energies will be computed in this thesis.
Both the 2N input and the 2N+3N(NO2B) output are JT-coupled and stored in an `pAntoine`-specific binary file format. These binary files only contain the matrix element values $\left\langle ab; JT \middle| v^{2N} \middle| cd; JT \right\rangle$ themselves. This means that `pyNO2B` must generate both a list holding the configuration a, b, c, d, J, T for each matrix element, and a single-particle basis listing the quantum numbers (n_i, l_i, j_i) for to the single-particle states specified by a,b,c,d. The ordering of elements in these lists are identical to the ones used by `pAntoine`. Naturally, larger values of N_{max} result in longer lists.
The 3N interaction is expressed in an uncoupled basis and is stored in a file in the HDF5 format [17]. In contrast to the 2N input file, this file contains all configura-

tion lists and bases needed to match matrix element values with the corresponding quantum numbers.

`pyNO2B` uses the following steps to arrive at the end result:

- The single-particle (SP) basis and configuration list used in the 2N and 2N+3N(NO2B) files are generated.
- For each 2N matrix element $\left\langle ab; JT \middle| V^{2N} \middle| cd, JT \right\rangle$ in the 2N input file:
  1. The values of a,b,c,d,J, T are looked up in the configuration list, and the corresponding quantum numbers $(n_{i=a,b,c,d}, l_i, j_i)$ are looked up in the SP basis.
  2. We are now ready to compute the JT-coupled NO2B element corresponding to a,b,c,d. This is done using the sum (2.33). For each term in the sum:
     (a) The Clebsch-Gordan coefficients are computed.
     (b) The m-scheme NO2B matrix element is calculated by summing the 2N, 1N and 0N contributions. This is described further in Section 3.2.1.
- The JT-coupled NO2B element is added to the 2N element and written to the output file.

One might add that in the above procedure the same m-scheme elements will be calculated repeatedly. Although this is not a huge problem when $N_{max} \leq 6$, an alternative approach must be used in larger model spaces.

3.2 Further details

3.2.1 NO2B m-scheme matrix elements

The matrix elements in the 3N interaction file is divided into different *data splits*, where each data split corresponds to a specific set of values of the conserved quantities $M_T = t_{za} + t_{zb} + t_{zc}$ and $M = m_a + m_b + m_c$. Altogether, the 3N interaction file contains the following parts:

1. Single-particle (SP) basis listing basis states $|i\rangle = |n_i, l_i, j_i, m_i, t_{zi}\rangle$.
2. Many-body (MB) basis listing three-particle states $|ijk\rangle$, where i,j,k are indices in the SP basis.
3. Each datasplit contains:
   - List of configurations (n, m) where n and m are the MB indices corresponding to the bra and ket states of the matrix element, respectively.
   - List of matrix elements, where the l^{th} element corresponds to the l^{th} configuration in the configuration list.

To calculate the m-scheme NO2B matrix elements we must be able to compute the

sums over the hole states (v, v_{ps}, v_{pqst}) as defined in (2.26)–(2.28):

$$v_{pqst} = \sum_i \langle pqi|\hat{v}^{3N}|sti\rangle$$
$$v_{ps} = \sum_{ij} \langle pij|\hat{v}^{3N}|sij\rangle = 2\sum_{i<j} \langle pij|\hat{v}^{3N}|sij\rangle$$
$$v = \frac{1}{6}\sum_{ijk} \langle ijk|\hat{v}^{3N}|ijk\rangle = \sum_{i<j<k} \langle ijk|\hat{v}^{3N}|ijk\rangle$$

Note that the by rewriting v_{ps} and v as above we avoid having to add identical terms (eg. $\langle pij|\hat{v}^{3N}|sij\rangle = \langle pji|\hat{v}^{3N}|sji\rangle$) multiple times, thus saving time.
v_{pqst} is computed as below. v and v_{ps} are calculated in an almost identical fashion.

- The single-particle states p,q,s,t corresponding to $(n_{i=a,b,c,d}, l_i, j_i, m_i, t_{zi})$ are looked up in the SP-basis in the 3N interaction file.
- For each hole state i:
  1. The data split indices corresponding to $|pqi\rangle$ and $|sti\rangle$ are computed. If they differ $\langle pqi|\hat{v}^{3N}|sti\rangle$ must be 0 and can be skipped.
  2. MB basis indices n and m corresponding to $|pqi\rangle$ and $|sti\rangle$, respectively, are looked up.
  3. The configuration index l corresponding to (n, m) is retrieved.
  4. The l^{th} matrix element is added to the sum.

3.2.2 Search algorithms

As seen above, calculating v_{pqst}, v_{ps} and v involves repeatedly searching the 3N input file for matching indices. Since the number of configurations and MB basis states is large, even for moderate values of N_{max}, the use of efficient search algorithms is imperative. As an example, there number of MB states is 51328 in the $N_{max} = 6$ case. Fortunately both the configurations and the MB basis states are already sorted in a specific order, meaning that we can use a binary search algorithm. The worst-case running time of a binary search is $O(\log n)$, which is significantly better than the linear $O(n)$ running time of a linear search.

3.2.3 External modules

`pyNO2B` mostly uses modules from the Python Standard Library. The two sole exceptions are the `h5py` module [4], which is used to read the HDF5 file format, and the `SymPy` module [16], which is used to compute the Clebsch-Gordan coefficients.

4
Results

The `pyNO2B` code was tested for helium-4 and $N_{max} = 0, 2, 4, 6$. The choice of helium-4 is obvious — the single-reference NO2B approximation is only applicable to closed-shell nuclei and helium-4 is the simplest example of such a system. The interaction used was NNLOsat [6], which is derived from chiral effective field theory and features both 2N and 3N interactions. To benchmark the results they were checked with the `ncsd` code [12], a many-body code capable of including both 2N and 3N interactions fully.

4.1 Ground state energies of helium-4

Ground state energies of helium-4 were computed using `pAntoine` for $N_{max} = 0, 2, 4, 6$ and for the following interactions: The plain 2N interaction, the plain interaction with the NO0B term added, with the NO1B terms added, and finally with the full NO2B approximation added. For each N_{max} a reference value was also calculated from the full 2N+3N interaction using `ncsd`. In all cases the HO frequency $\hbar\omega = 22$ MeV is used. The results are presented in Table 4.1.

		2N+3N				
N_{max}	2N	NO0B	NO1B	NO2B	Full	Rel. error
0	-17.06463	-13.88235	-13.88235	-13.88235	-13.8845	0.015%
2	-19.95847	-16.77619	-16.53317	-18.72536	-18.5570	0.91%
4	-23.88394	-20.70166	-20.47555	-24.11923	-23.7846	1.41%
6	-25.56324	-22.38095	-22.13663	-26.99404	-26.6596	1.25%

Table 4.1: Ground state energies of helium-4 in MeV, calculated at various N_{max} with $\hbar\omega = 22$ MeV. `ncsd` was used for the full 2N+3N calculations, whereas the other columns were computed using `pAntoine`. The last column is the relative error of the 2N+3N(NO2B) results compared to the full 2N+3N calculations.

Including the 3N interaction has been shown to result in a ∼10% [11] increase in the binding energy. The calculations with `ncsd` demonstrates, however, that for small model spaces the opposite is true — the binding energy actually decreases.
For $N_{max} = 0$ both the NO0B, the NO1B and the NO2B approximations give the same result, which is very close to the reference value. This can be understood by noting that the only configuration in the $N_{max} = 0$ model space is the Fermi state. As we observed in the introduction all interactions between the Fermi state and itself are included in the 0N term, which is retained in all three approximations. The fact

that we do not get a perfect agreement can probably be attributed to rounding errors.
As expected the NO0B term introduces a constant shift in the ground state energies. With the exception of the $N_{max} = 0$ case, this is actually farther from the reference value than the result of the pure 2N interaction itself. This is also true, although to a slightly smaller extent, when the NO1B approximation is applied. It is only when the full NO2B approximation is employed that we get close to the reference values in any real sense.
Previous studies [13] have shown that the errors introduced by NO2B approximation is in the order of 1–2% for converged (i.e. for large values of N_{max}) calculations of the helium-4 ground state energy. More precisely, an overbinding of 0.3–0.6 MeV is observed. Although our results are far from converged, we note that relative errors for Nmax = 2,4,6 lie within the 1%–2% range. Furthermore the absolute error is 0.33463 MeV and 0.33444 MeV, respectively, suggesting that the overbinding stabilises at slightly above 0.3 MeV. We can therefore conclude that our limited results are in line with expectations, although more results might be needed for a final verdict.

5

Conclusion and Outlook

In this thesis we have provided a full derivation of the single-reference NO2B approximation together with the necessary formalism. A simple Python implementation `pyNO2B` of this scheme has also been described. The goal of this implementation was to test the approximation in small model spaces. As a benchmark, `pyNO2B` was applied to helium-4 for $N_{max} = 0, 2, 4, 6$ and compared to calculations using the full 3N interaction. The results were favourable and in line with previously published results. More specifically we have shown that the main contribution of 3N forces to the ground-state energy of helium-4 can be accounted for using the NO2B approximation — i.e. with an effective 2N force. In fact, the neglect of the remaining (non-reducible) 3N part was shown to result in just 1-2% relative error in the final result.

Since `pyNO2B` code was written with only limited attention paid to performance it is too slow to be used in model spaces larger than $N_{max} = 6$. There are several ways to improve this situation. The most obvious is to pre-calculate the m-scheme matrix elements to avoid wasting time on repeating calculations. In the same token Clebsch-Gordan coefficients could also be cached. This approach would probably reduce the running time significantly, but to reach large model spaces additional steps may have to be taken. Being a dynamically-typed interpreted language, Python programs are often slower than implementations in other languages. Rewriting `pyNO2B` in C would most likely improve the performance dramatically. Finally, the program is easy to parallelise since the problem is embarrassingly parallel — all matrix elements can be computed independently from each other.

The single-reference NO2B approximation presented in this thesis is only applicable to closed-shell nuclei. By using a generalised multi-reference normal ordering as defined in [8] the multi-reference normal-ordered two-body (MR-NO2B) approximation can be introduced. This can be applied to both open-shell nuclei and nuclei in excited states as demonstrated in [7].

In conclusion, the single-reference NO2B approximation enables us to study the effects of the 3N interaction on closed-shell nuclei for much larger systems and model spaces than a full inclusion would allow. This thesis has provided a full derivation of this approximation and demonstrated that it can be implemented in a relatively simple program.

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