BENCHMARKING ISOSPIN SYMMETRY BREAKING IN AB INITIO NUCLEAR THEORY VIA THE ISOBARIC MULTIPLETT MASS EQUATION IN $T = 1$ SUPERALLOWED $\beta$ DECAY SYSTEMS

by

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A thesis submitted to the Faculty and the Board of Trustees of the Colorado School of Mines in partial fulfillment of the requirements for the degree of Master of Science (Applied Physics).

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ABSTRACT

Searching for physics Beyond the Standard Model (BSM) has become a central focus in physics research over the past few decades. One way to do this is through precision measurements of superallowed $0^+ \rightarrow 0^+$ Fermi $\beta$ decay. These decays give the most precise measurements of the vector coupling constant of the weak interaction, an important step in calculating the up-down element of the Cabibbo-Kobayashi-Maskawa (CKM) matrix. CKM unitarity, if broken, would imply significant physics BSM. However, the extraction of the vector coupling constant assumes perfect isospin symmetry in nuclei, requiring theoretical isospin symmetry breaking (ISB) corrections to be applied.

The ISB corrections can be calculated using \textit{ab initio} nuclear many body methods using interactions from chiral effective field theory. However, before these corrections can be used reliably for BSM physics searches, they must be benchmarked against known results. In this Thesis, \textit{ab initio} methods are used to calculate the coefficients of the isobaric multiplet mass equation (IMME) for $T = 1$ superallowed $0^+ \rightarrow 0^+$ Fermi $\beta$ decay systems. The implications of the IMME coefficients to ISB corrections are also discussed.
"It doesn’t matter how beautiful your theory is, it doesn’t matter how smart you are. If it doesn’t agree with experiment, it’s wrong."

- Richard P. Feynman
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LIST OF ABBREVIATIONS

Beyond the Standard Model ............................................. BSM
Cabibbo-Kobayashi-Maskawa ........................................... CKM
Chiral Effective Field Theory .......................................... \chiEFT
Conserved Vector Current ............................................... CVC
Effective Field Theory ................................................... EFT
Electron Capture .......................................................... EC
In Medium Similarity Renormalization Group ......................... IMSRG
Isobaric Analogue States ................................................ IAS
Isobaric Analogue Triplet ............................................... IAT
Isobaric Multiplet Mass Equation ..................................... IMME
Isospin Symmetry Breaking ............................................. ISB
Quantum Chromodynamics ............................................. QCD
Quantum Electrodynamics .............................................. QED
Quantum Field Theory ................................................... QFT
Similarity Renormalization Group ..................................... SRG
Standard Model ........................................................... SM
Valence-Space In-Medium Similarity Renormalization Group .......... VS-IMSRG
Woods Saxon ............................................................... WS
ACKNOWLEDGMENTS

First of all I would like to thank my advisors Dr. Kyle Leach and Dr. Jason Holt for their guidance, supervision, and support throughout the year. The environment that you provided allowed me to learn and grow throughout the entire process. I look forward to continue working with both of you in the future.

Additionally I would like to thank Dr. Ragnar Stroberg for the countless hours spent discussing various topics, the large number of poorly worded or misguided questions that you answered, and all the other guidance and direction you provided for me. I would not have gotten anywhere near the level of understanding or amount of work done that I did without your help.

For many things, I would like to thank Madeleine Hanley. Throughout the entire year you were supportive and encouraging, were always ready to help and never seemed to mind when I complained about any snags I hit when doing this work. Thank you for that, but also for giving me a great reason to take frequent, very enjoyable trips to Seattle. None of this work could have been completed without you. Thank you very much.

I would like to thank all of those with whom I share an office for their support both in my research and personally. Getting to share this experience with all of you made it much more rewarding, and the numerous lunch breaks and random, off-topic discussions helped make the atmosphere something I will never forget. In particular, I would like to acknowledge Connor Pierce, Brooks Venuti, Kellen Malone, and Spencer Fretwell for their support and friendship throughout the entire process. I would also like to thank those who helped me with the programming aspects of my work, including Michael Bainbridge, Jon Ringuette, Connor Natzke, and Connor Bray among others. Without you I never would have been able to finish my work on time, or learn nearly as much about computers as I did.
Last, but certainly not least I would like to thank my family. I would like to thank my parents, Scott and Becky Martin, for their unwavering support and understanding. I would also like to thank my grandparents, who always took an interest in my work and asked some extremely difficult and important questions that I had not considered. Finally, I would like to thank my siblings for their input both in the work being done as well as in my life.

Thank you all very much. I could not have done this without all of you.
1.1 The Standard Model of Particle Physics

The Standard Model (SM) is the underlying framework, based in quantum field theory (QFT), which describes the electromagnetic, weak nuclear, and strong nuclear interactions. While the electromagnetic interaction, like the gravitational interaction, acts at all distances, both the weak and strong nuclear interactions are only relevant at extremely short distances, such as those within the diameter of an atomic nucleus \((r \approx 10 \text{ fm})\) [1]. To date, the SM has been one of the most successful scientific theories due to both its consistency with the results of nuclear and particle physics experiments, but also its ability to predict new physics yet to be measured. One prominent example of this was the prediction of the Higgs boson in 1964 [2, 3], and its subsequent discovery by the ATLAS and CMS collaborations in 2012 [4].

1.1.1 The Particles of the Standard Model

In the SM there exist seventeen fundamental fields, each with a corresponding particle resulting from excitations of the field. These particles are shown in Figure 1.1, which organizes the particles systematically. These can be broken down into two categories: Fermions and Bosons. Fermions are matter particles, have spin of \(\frac{1}{2}\), and obey the Pauli exclusion principle, while Bosons are charge carriers which mediate the three gauge interactions, have integer spin, and are not required to obey the Pauli exclusion principle.

Fermions can be further subdivided into quarks and leptons, each having three generations with increasing mass. The three leftmost columns in Figure 1.1 correspond to the first, second, and third generations of these Fermions, decreasing in stability with increasing mass. The bottom row is composed of neutrinos, which carry no electric charge and are affected by the weak interaction only. The other row of leptons, the second from the bottom, are the electron, muon, and tau particles which have an electric charge of \(-1e\), where \(e\) is the
fundamental electric charge. This row of Fermions feel both the weak and electromagnetic interactions. The quarks, the top two rows on the left side of Figure 1.1, feel all three interactions in the SM, and it is the first generation of these quarks which are the building blocks of nuclear matter.

Bosons can also be further subdivided, though the division only separates one particle from the other four. This division is between scalar and gauge Bosons, the former of which consists only of the Higgs Boson. The Higgs Boson is the field responsible for giving mass to the quarks, top row of leptons, and the $W^\pm$ and $Z$ Bosons in the SM [3]. In fact, the only mass in the SM which is not derived from a coupling from the Higgs field is the Higgs Boson itself, though other particles, such as neutrinos, have mass not predicted by the SM. The mass of the Higgs comes from the shape of the Higgs potential [5].

The gauge bosons mediate the three interactions within the SM. The gluon, of which there are eight, mediates the strong interaction between quarks. As discussed in [6], it is interactions between quarks and their surrounding medium, partially filled with gluons,
which accounts for most of the observable mass in a nucleon. The weak interaction is mediated by the $W^\pm$ and $Z$ bosons, while the electromagnetic interaction is mediated by the photon.

### 1.1.2 The Cabibbo-Kobayashi-Maskawa Matrix

In the SM, the weak interaction and mass eigenstates of the quarks are not equal but are related through a unitary transformation. The matrix representation of this transformation is known as the Cabibbo-Kobayashi-Maskawa (CKM) matrix, developed by Cabibbo in 1963 [7], and updated by Kobayashi and Maskawa in 1973 [8]. The current form of the CKM matrix is shown in Eq. 1.1

\[
\begin{bmatrix}
  d' \\
  s' \\
  b'
\end{bmatrix} =
\begin{bmatrix}
  V_{ud} & V_{us} & V_{ub} \\
  V_{cd} & V_{cs} & V_{cb} \\
  V_{td} & V_{ts} & V_{tb}
\end{bmatrix}
\begin{bmatrix}
  d \\
  s \\
  b
\end{bmatrix},
\]

(1.1)

where the letters represent quarks in the SM.

Because a unitary transformation is simply a change of basis and does not change the underlying physics, unitarity of the CKM matrix is essential for support of the SM. This makes testing CKM unitarity a test of the SM, and in particular, a failure of CKM unitarity would imply physics Beyond the SM (BSM).

In order to test CKM unitarity, numerical values for the elements of the CKM matrix need to be determined. These can be determined experimentally in a variety of methods [9–11], and at the time of writing, the CKM elements are

\[
\begin{bmatrix}
  |V_{ud}| & |V_{us}| & |V_{ub}| \\
  |V_{cd}| & |V_{cs}| & |V_{cb}| \\
  |V_{td}| & |V_{ts}| & |V_{tb}|
\end{bmatrix} =
\begin{bmatrix}
  0.97420(21) & 0.2243(5) & 0.00394(36) \\
  0.218(4) & 0.997(17) & 0.0422(8) \\
  0.0081(5) & 0.0394(23) & 1.019(25)
\end{bmatrix},
\]

(1.2)

where only the magnitudes are shown. More details on the CKM matrix and it’s elements can be found in [11].

Because of the relative precision of the elements of the CKM matrix, the top row is typically used for the test, needing to satisfy Eq. 1.3 to satisfy matrix unitarity.

\[
|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 1
\]

(1.3)
The up-down element of the CKM matrix, $V_{ud}$, is the most precisely known element and its magnitude dominates the calculation of unitarity. This matrix element connects the up and down quarks, and can be measured experimentally using nuclear processes including both of these. Specifically, $V_{ud}$ can be measured through pion decay, the decay of quark-antiquark pairs, as well as a particular type of nuclear decay of larger systems known as superallowed Fermi $\beta$ decays \cite{11}, which is the focus of this Thesis and is discussed in more details in the following pages.

1.2 Nuclear Decay

Nuclear decay is a statistical process by which the atomic nucleus emits radiation and transitions to an energetically favourable state. The decay constant, $\lambda$, is used to characterize nuclear decay rates

$$\frac{dN(t)}{dt} = -\lambda N(t), \quad (1.4)$$

where $N(t)$ is the number of remaining nuclei present at any given time. Eq. 1.4 can be integrated to give the number of nuclei present as a function of time and the decay constant

$$N(t) = N(0)e^{-\lambda t}. \quad (1.5)$$

The half life, $t_{1/2}$, or statistical average length of time it takes half of a radioactive sample to decay, is directly related to the decay constant as

$$t_{1/2} = \frac{\ln(2)}{\lambda}. \quad (1.6)$$

It is the half life of nuclear decay which can be measured experimentally to extremely high precision. However, a given nucleus can decay in multiple ways, each having their own half life. The branching ratio,

$$B_n = \frac{\lambda_n}{\lambda}, \quad (1.7)$$

where $\lambda_n$ is the decay constant for the $n^{th}$ decay mode, gives the fraction by which a nucleus decays by a specific decay mode compared to the total decay rate.
1.2.1 Nuclear $\beta$ Decay

Nuclear $\beta$ decay is the decay mode by which nuclei lower their total energy and become more bound by exchanging a nucleon for another (i.e. neutron to proton or proton to neutron). This process can happen in three ways: $\beta^-$ decay, $\beta^+$ decay, and electron capture (EC). $\beta^-$ decay is the exchange of a bound neutron into a proton

$$A_Z X_N \to A_{Z+1} Y_{N-1} + e^- + \bar{\nu}_e,$$

where $X$ and $Y$ represent the parent and daughter nuclei respectively, and an electron and anti-electron neutrino are emitted to preserve lepton number, charge, and angular momentum. This decay mode most commonly occurs on the neutron rich side of the nuclear chart where there is a relative surplus of neutrons.

$\beta^+$ decay is the exchange of a bound proton for a neutron,

$$A_Z X_N \to A_{Z-1} W_{N+1} + e^+ + \nu_e$$

with the emission of a positron and an electron neutrino. Electron capture (EC) decay competes with $\beta^+$ decay as the parent and daughter nuclei are the same, but the emitted positron in $\beta^+$ decay becomes an orbital electron of the parent nucleus, as shown in Eq. 1.10. In EC decay, the wavefunctions of the nucleus and orbital electrons overlap allowing for the capture of one of these orbital electrons.

$$A_Z X_N + e^- \to A_{Z-1} W_{N+1} + \nu_e$$

As energy must be released in the process in order for the decay mode to result in an increased binding, the decay energy, known as the $Q$-value, must be positive. $Q$-values can be calculated for $\beta^-$, $\beta^+$, and EC decays using Eqns. 1.11, 1.12, and 1.13 respectively [12]

$$Q_{\beta^-} = [m (A_Z X_N) - m (A_{Z+1} Y_{N-1})] c^2$$

$$Q_{\beta^+} = [m (A_Z X_N) - m (A_{Z-1} W_{N+1}) - 2m_e] c^2$$

$$Q_{EC} = [m (A_Z X_N) - m (A_{Z-1} W_{N+1})] c^2 - B_a,$$
where \( m (^{A}_Z X_N) \) corresponds to the neutral atomic mass of element \( X \) with \( A \) nucleons, \( N \) neutrons, and \( Z \) protons, \( m_e \) is the mass of the electron, and \( B_a \) is the atomic binding energy of the captured electron. The \(-2m_e c^2\) term in \( Q_{\beta^+}\) results in there being many nuclei which only undergo EC decay, despite the energy of a daughter of \( \beta^+ \) decay being of lower energy [12].

\( \beta \) decay still requires a conservation of angular momentum for the entire system,

\[
\vec{J}_P = \vec{J}_D + \vec{J}_\beta,
\]

where \( \vec{J} \) represents the total angular momentum, and the subscripts \( P, D, \) and \( \beta \) represent the parent nucleus, daughter nucleus, and electron (positron) and anti-neutrino (neutrino) from the \( \beta^+ (\beta^-) \) decay respectively. The total angular momentum of a state can be calculated as the sum of its orbital angular momentum (\( \vec{L} \)) and spin (\( \vec{S} \))

\[
\vec{J} = \vec{L} + \vec{S},
\]

and \( S_\beta \) can be split into two independent pieces

\[
\vec{S}_\beta = \vec{S}_e + \vec{S}_\nu.
\]

As there are two particle contributing to the total spin of the emitted particles from the \( \beta \) decay and they are both Fermions, the system can have a value of either 0 or 1. If \( S_\beta = 0 \), the decay is referred to as a Fermi decay, and if \( S_\beta = 1 \) the decay is referred to as a Gamow-Teller decay. The range of orbital angular momenta possible allow for another classification of decay, summarized in Table 1.1.

Table 1.1: Classification of \( \beta \) decay by orbital angular momentum [12]

<table>
<thead>
<tr>
<th>( L_\beta )</th>
<th>Type of Decay</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Allowed</td>
</tr>
<tr>
<td>1</td>
<td>First Forbidden</td>
</tr>
<tr>
<td>2</td>
<td>Second Forbidden</td>
</tr>
<tr>
<td>3</td>
<td>Third Forbidden</td>
</tr>
<tr>
<td>4</td>
<td>Fourth Forbidden</td>
</tr>
</tbody>
</table>
Using these two naming classifications, a decay where the emitted particles have total orbital angular momentum and spin of 1 and 2 respectively would be classified as a Second Forbidden Gamow-Teller decay. This Thesis focuses on superallowed Fermi β decay, a special classification of Allowed Fermi decays

1.2.2 Fermi Theory of β Decay

Though the modern understanding of the weak interaction did not arise until the 1960s [5], in 1934, based on Pauli’s proposed neutrino, Fermi developed a theory of β decay, the foundations of which are still relevant at the time of writing of this Thesis [13]. In Fermi’s theory, the force which governs decay is weak compared to the force which creates the nuclear states, thus leading to the possibility of a perturbative expansion of the transition operator [12]. This allows the transition rate for decay to be written

\[ \lambda = \frac{2\pi}{\hbar} |M_{fi}|^2 \frac{dn}{dE}, \]

Eq. 1.17 is known as Fermi’s Golden Rule [12]. This accounts for the electron (positron) and anti-neutrino (neutrino) being emitted for \( \beta^- (\beta^+) \) decay, as well as the daughter nucleus. Using this as a starting point, and expanding out the density of final states (see Appendix A for details), the decay constant can be written as

\[ \lambda = g^2 |M_{fi}|^2 \frac{m_e^5 c^4}{2\pi^3 \hbar^7} f(Z_D, E), \]

Eq. 1.18

where \( g \) is the coupling constant, \( f(Z_D, E) \) is the dimensionless phase integral

\[ f = f(Z_D, E) = \frac{1}{(m_e c)^3 (m_e c^2)^2} \int F(Z_D, p_e) p_e^2 (E - E_e)^2 dp_e, \]

where \( F(Z_D, p_e) \) is the Fermi function [12].

The transition matrix \( |M_{fi}|^2 \) can be further broken down based on empirical evidence into two coupling constants and two independent transition matrices for Fermi and Gamow-Teller decays. This is because the weak interaction has been shown to have only vector and
axial-vector contributions [14].

\[ |M_{fi}|^2 = g^2 \left|M'_{fi}\right|^2 \]
\[ = G_V^2 \left|M'_{fi}(F)\right|^2 + G_A^2 \left|M'_{fi}(GT)\right|^2 \]  \hspace{0.5cm} (1.20)

In Eq. 1.20, which details how the transition matrix element for $\beta$ decay can be broken down, $G_V$ is the vector coupling constant and $G_A$ is the axial-vector coupling constant. Because this Thesis deals with pure Fermi decay, and specifically superallowed $0^+ \rightarrow 0^+$ Fermi $\beta$ decay, the matrix element for Gamow-Teller decay is identically zero and does not contribute, allowing the decay constant to be written as a function of only the vector coupling constant and the Fermi matrix element

\[ \lambda = \frac{G_V^2 \left|M'_{fi}(F)\right|^2 m^2 c^4}{2\pi^3 \hbar^7} f(Z_D, E). \]  \hspace{0.5cm} (1.21)

Multiplying Eqs. 1.6 and 1.21 together gives the $\beta$ decay $ft$ value

\[ ft = \frac{2\pi^3 \hbar^7 \ln(2)}{m_e^2 c^4 \left(G_V^2 \left|M'_{fi}(F)\right|^2\right)}; \]  \hspace{0.5cm} (1.22)

a value which allows all types of $\beta$ decay to be compared.

As the $ft$ value can be experimentally obtained, this allows for the extraction of the vector coupling constant of the weak interaction, $G_V$.

1.2.3 Isospin, Isospin Symmetry, and Isobaric Analogue Triplets

As early as the 1930s, the two nucleon ($NN$) forces acting between proton-proton ($pp$) and neutron-neutron ($nn$) pairs were known to be extremely similar (e.g. [15]). This apparent symmetry of the strong interaction between $pp$ and $nn$ forces prompted Heisenberg [16] and Wigner [17] to introduce a concept called isospin symmetry, where protons and neutrons are treated as a single particle, the nucleon, with a different projection of a quantity called isospin. Both nucleons are given an isospin ($t$) of $\frac{1}{2}$, but different $z$ projections ($t_z$) of the quantity. The assigned projections are $+\frac{1}{2}$ and $-\frac{1}{2}$ for the neutron and proton respectively.
Mathematically, these states can be written as shown in Eqs. 1.23 and 1.24.

\[ |n\rangle = \left| t = \frac{1}{2}, t_z = +\frac{1}{2} \right\rangle \]  
(1.23)

\[ |p\rangle = \left| t = \frac{1}{2}, t_z = -\frac{1}{2} \right\rangle \]  
(1.24)

The combination of nucleons adds isospin to create total isospin projection \( (T_z) \) analogously to the addition of angular momentum. This means that for a two nucleon system with total isospin \( T = 1 \), there are three possible projection states. These states are summarized in Figure 1.2, where it becomes obvious that for \( T = 0 \) systems there exists an isospin singlet, and for \( T = 1 \) systems there exists an isospin triplet.

\[ T_z \]

(a) \( T = 0 \)

(b) \( T = 1 \)

Figure 1.2: Graphical representation of \( T = 0 \) and \( T = 1 \) states and their \( z \) projections

The isospin singlet and triplet states shown in Figure 1.2 can be written with the convention \( |T, T_z\rangle \) as

\[ |0, 0\rangle = \frac{1}{\sqrt{2}} (|np\rangle - |pn\rangle) , \]  
(1.25)
These states show the same properties as angular momentum singlets and triplets; under the exchange of particles the singlets are anti-symmetric and triplets are symmetric.

Extending the concept of total isospin to an $A$-nucleon system with $N$ neutrons and $Z$ protons, the total isospin projection can be calculated as

$$T_z = \frac{1}{2} (N - Z).$$

The tendency towards nuclear symmetry indicates that the ground state of almost all nuclei have total isospin equal to the absolute value of the $z$ projection ($T = |T_z|$) [12, 18]. Though the ground state of an $N = Z$ nucleus will have $T_z = 0$, this state can correspond to either $T = 0$ or $T = 1$. In fact, for a set of three nuclei or arbitrary but equal $A$ and centred around the $N = Z$ line, there is a single $T = 0$ state for the $N = Z$ nucleus and a triplet of $T = 1$ states.

If a perfect symmetry of isospin exists, meaning that there is no distinction between the proton and neutron under nuclear interactions, then the three $T = 1$ states would be perfectly degenerate [12]. In reality, isospin symmetry is not perfect, and is violated primarily by the Coulomb interactions [15], though isospin symmetry breaking (ISB) terms of non-negligible magnitude also exist in the strong interaction [19]. This lack of perfect isospin symmetry makes the three $T = 1$ states, known as an isobaric analogue triplet (IAT), non-degenerate.

Because states in the IAT are non-degenerate yet still lie along an isobar, they are connected to each other via $\beta$ decay. For the $T = 1$ IATs of interest in this Thesis, the states are connected via superallowed Fermi $\beta$ decay. In these specific transitions the wavefunctions of the parent and daughter nucleus are identical except for the exchange of a nucleon, meaning that an isospin ladder operator, $\hat{T}^\pm$, can be used to connect the states and calculate the
Figure 1.3: Three nuclei centred around \( N = Z \) with the isospin singlet and isospin triplet states shown. The highlighted states correspond to an isobaric analogue triplet transition matrix element.

The rules of isospin are the same as those for angular momentum, meaning the length of an isospin vector can be written

\[
|t| = \sqrt{t(t+1)}\hbar,\tag{1.28}
\]

where \( t \) is an isospin vector and \( t \) is the isospin quantum number [12]. Additionally, the effect of applying an isospin ladder operator onto an arbitrary ket can be done analytically for \( \beta^\pm \) decay.

\[
\hat{T}^\pm |T, T_z\rangle = \sqrt{(T \mp T_z)(T \pm T_z + 1)} |T, T_z \pm 1\rangle \tag{1.29}
\]

Using this ladder operator as the transition element for the \textit{superallowed} \( \beta \) decay for the \( T = 1 \) IAT, the matrix element can be analytically solved as

\[
\left| \mathcal{M}_{fi}(F) \right|^2 = \left| \langle T, T_z \pm 1 | \hat{T}^\pm |T, T_z\rangle \right|^2 = (T \mp T_z)(T \pm T_z + 1)
\]

\[
\left| \mathcal{M}_{fi}(F)_{T_z=-1 \rightarrow T_z=0} \right|^2 = (1 + 1)(1 - 1 + 1) = 2 \tag{1.30}
\]

\[
\left| \mathcal{M}_{fi}(F)_{T_z=0 \rightarrow T_z=+1} \right|^2 = (1 - 0)(1 + 0 + 1) = 2. \tag{1.31}
\]
That both matrix elements come out to exactly 2 and be independent of any nuclear wave functions is significant because it allows the \( \beta \) decay \( ft \) value (Eq. 1.22) to be written, for the superallowed \( \beta \) decays between \( T = 1 \) isobaric analogue states (IAS), in terms of constants [20]

\[
ft = \frac{2\pi^3\hbar^7 \ln(2)}{m_e^5 c^4 (2G_F^2)}.
\]

(1.33)

### 1.2.4 Corrected \( Ft \) Values

The \( \beta \) decay \( ft \) value is an experimentally determined measure of the decay and can be extracted using experimental data to high precision [20]. \( \beta \) decay \( ft \) values can span orders of magnitude from approximately \( 10^3 \) to \( 10^{20} \) s, and values are often quoted in \( \log_{10}(ft) \) for that reason [12]. Though the range of \( ft \) values is significantly smaller for allowed decays, the range is much larger than for superallowed decay. In fact, the \( ft \) values for superallowed decay are expected to be nearly constant as predicted by Eq. 1.33. \( ft \) values for allowed and superallowed decay can be seen graphically in Figure 1.4.

In Figure 1.4, it appears that the \( ft \) values of the superallowed decays are constant, which coincides nicely with Eq. 1.33 where the \( ft \) value for superallowed decays was written as a collection of constants. This constant value, while not necessarily intuitive, is predicted by the Conserved Vector Current (CVC) hypothesis [20, 24].

Although this is extremely promising, Eq. 1.33 was derived assuming perfect isospin symmetry. Zooming in on Figure 1.4 and looking only at the superallowed \( ft \) values, Figure 1.5 can be produced, which shows a clear deviation from a constant value. While there is deviation from a constant value, the deviation is relatively small when compared to the \( ft \) values themselves, so the assumptions made in the derivation of Eq. 1.33 can be corrected using small corrections rather than an entire re-working of the Fermi theory. These corrections lead to what is known as the corrected \( ft \) value, or \( Ft \) value. The \( Ft \) value corrects the experimental \( ft \) value for radiative and ISB corrections [20] and is the constant value
Figure 1.4: $\beta$ decay $ft$ values for selected allowed and superallowed decays. Sample of allowed taken at random with data from [21] and $ft$ values calculated using [22]. Superallowed decays taken from [20] and include the most precise 14 $ft$ measurements to date. $^{10}$C includes the recent half-life measurement from [23] as well as theoretical corrections from [20].

Figure 1.5: $\beta$ decay $ft$ values for the 14 most precisely measured superallowed decays. Data taken from [20] as well as $T_{1/2}(^{10}$C$)$ data taken from [23].
predicted by the CVC. The $F_t$ value can be parameterized as,

$$F_t = f_t (1 + \delta'_R)(1 - \delta_C) = \frac{2\pi^3 h^7 \ln(2)}{m^5_e c^4 (2G^2_F)(1 + \Delta Y_R)},$$  \hfill (1.34)

where $\delta'_R$ is a transition-dependent radiative correction, $\delta_C$ is the ISB correction, and $\Delta Y_R$ is a transition-independent radiative correction. The $F_t$ value, shown graphically in Figure 1.6, becomes a constant value across the superallowed decays.

![Figure 1.6: $F_t$ values for superallowed $\beta$ decay transitions.](image)

Figure 1.6: $\beta$ decay $F_t$ value calculated using the 14 most precisely measured superallowed decays. Data taken from [20] as well as $T_{1/2}^{^{10}\text{C}}$ taken from [23].

### 1.2.5 Theoretical Corrections

Despite the precision of the $F_t$ value, there is still ongoing work, both theoretically and experimentally, to increase this precision by understanding better the theoretical corrections (e.g. [20, 25]). Of the three theoretical corrections in Eq. 1.34, there are two radiative corrections and one ISB correction. The two radiative corrections, which are not a point of emphasis in this Thesis, correct for radiative processes in $\beta$ decay, such as bremsstrahlung radiation [20], and are suppressed by a factor of $\alpha = \frac{1}{137}$ giving their magnitude on the order of $\sim 1\%$. The first of these terms, $\delta'_R$, includes corrections from long range, low energy
effects such as the bremsstrahlung radiation, and as a nucleus dependent correction needs to be applied separately for each nucleus. This correction depends only on the electron’s wavefunction and the central potential created by the daughter nucleus, and therefore is independent of complex nuclear structure calculations [26]. The second radiative correction is the transition-independent correction which depends on short range, high energy radiative effects. As this correction, \( \Delta V_R = 2.361(38) \% \) [26], stems from free quark Lagrangians [20] and short distance loop effects [27], it is considered constant for all nuclei.

The final correction, the ISB correction, accounts for the lack of perfect isospin symmetry in the interactions between nucleons as well as in the nucleon wavefunctions. As discussed in Section 1.2.3, ISB in the nuclear Hamiltonian comes both from the Coulomb interaction as well as strong charge dependent terms, and therefore isospin is not a perfect symmetry. This lack of perfect symmetry is an important consideration as the matrix element for Fermi decay, \( |\mathcal{M}_{fi}(F)|^2 \), calculated to be equal to 2 for both superallowed Fermi decays, is calculated under the assumption of perfect isospin symmetry.

In a more general sense, the Fermi matrix element, \( \mathcal{M}_{fi}(F) \), can be calculated by taking the expectation value of the isospin ladder operator with the initial and final states of the decay

\[
\mathcal{M}_{fi}(F) = \langle f | \hat{T}^\pm | i \rangle ,
\]

which can be rewritten in the second quantized form with creation and annihilation operators as

\[
\mathcal{M}_{fi}(F) = \sum_\alpha \langle f | a_\alpha^\dagger b_\alpha | i \rangle ,
\]

where \( a_\alpha^\dagger \) creates a neutron and \( b_\alpha \) annihilates a proton. Inserting a sum over all possible states \( \pi \)

\[
\mathcal{M}_{fi}(F) = \sum_{\alpha, \pi} \langle f | a_\alpha^\dagger \pi \rangle \langle \pi | b_\alpha | i \rangle ,
\]
allows for the Fermi matrix element, assuming perfect isospin symmetry, to be written as

\[ \mathcal{M}_{f_i}^0(F) = \sum_{\alpha,\pi} |\langle f | a^\dagger_\alpha | \pi \rangle|^2, \quad (1.38) \]

which is the matrix element equal to 2 discussed in Section 1.2.3. However, because this is not a perfect symmetry, an ISB correction needs to be applied, and is done so by studying the total matrix element squared compared to the square of the matrix element in 1.38

\[ |\mathcal{M}_{f_i}(F)|^2 = |\mathcal{M}_{f_i}^0(F)|^2 (1 - \delta_C). \quad (1.39) \]

This ISB correction, \( \delta_C \), is the same ISB correction used in the calculation of the \( \mathcal{F}t \) value in Eq. 1.34, and can be determined using a theoretical calculation of the Fermi matrix element \([28, 29]\) and Eq. 1.39.

### 1.2.6 Extraction of \( V_{ud} \) from the Superallowed Data

Because of the constancy of the \( \mathcal{F}t \) value, the vector coupling constant of the weak interaction, \( G_V \), is not calculated using individual \( \mathcal{F}t \) values, but rather a weighted average of the 14 most precise measurements (included in Figure 1.6). The vector coupling constant can be calculated using Eq. 1.40, which is a rearrangement of Eq. 1.34 with the \( \mathcal{F}t \) value replaced by the weighted average, \( \mathcal{F}t \)

\[ G_V = \frac{2\pi^3\hbar^7 \ln(2)}{m^2c^42\mathcal{F}t(1 + \Delta^V_R)}. \quad (1.40) \]

This calculation of \( G_V \) can be combined with the Fermi coupling constant, \( G_F \), measured through muon decay \([30]\), to calculate \( V_{ud} \)

\[ V_{ud} = \frac{G_V}{G_F}. \quad (1.41) \]

Using the global value of the Fermi coupling constant \([11]\),

\[ \frac{G_F}{(\hbar c)^3} = 1.1663787(6) \times 10^{-5}\text{GeV}^{-2}, \quad (1.42) \]
\( \mathcal{F} t \) is calculated using the measured \( \mathcal{F} t \) values presented in [20], and the updated half life of \(^{10}\text{C} \) in [23].

\[
\mathcal{F} t = 3072.29(61) \text{ s}
\] (1.43)

This gives a calculated \(|V_{ud}| \) value as

\[
|V_{ud}| = 0.97417(21).
\] (1.44)

\( V_{ud} \) is the most precisely measured value in the CKM matrix, and despite this, the large value causes the element to dominate the error budget of the top row sum.

\[
|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.99939(47) \] (1.45)

The error budget of \( V_{ud} \) itself is dominated by the theoretical corrections to the \( \mathcal{F} t \) calculation [20], and an increase in precision of these corrections using \textit{ab initio} methods allows for more stringent tests of the SM. Perhaps more important than the reduction of error bars though is that by using \textit{ab initio} methods to calculate the ISB correction, the central value will be better understood and therefore more reliable than if it were calculated using phenomenological methods.

The purpose of this Thesis is to begin benchmarking the ISB terms in \textit{ab initio} methods against experiment. Without first benchmarking ISB, the central value which can be calculated using \textit{ab initio} methods cannot be stated with any confidence.
CHAPTER 2
THEORETICAL METHODS

While the underlying theory explaining the electromagnetic interaction at the quantum scale is quantum electrodynamics (QED), the current theory of the strong interaction, quantum chromodynamics (QCD) is non-perturbative in the low energy regime and therefore cannot be used for the calculation of nuclear properties [31]. In fact, at the time of writing of this Thesis there is no mathematically consistent theoretical method for fully describing the nucleus.

Because there is no consistent theoretical method for the calculation of nuclear properties, many different methods are currently used to both explain experimental data and make predictions for yet-to-be measured quantities. These methods, at least in a shell model context, can be broadly split into two types:

1. Phenomenological, where basic principles such as the Woods-Saxon (WS) potential are used and fitting parameters adjusted to fit experimental data

2. Ab initio, a more mathematically consistent set of methods aiming to describe nuclear properties using a first-principles approach with limited fitting to experiment

This Thesis focuses on ab initio methods, and specifically chiral effective field theory (χEFT). χEFT is an effective field theory (EFT) based on Yukawa’s pion exchange model from 1934 [32]. Yukawa’s model with the addition of chiral symmetry in the 1990s [33] provides a mathematically consistent way to calculate nuclear properties, but is still imperfect and is still the subject of much research in theoretical nuclear physics [31].

Current research in ab initio nuclear theory includes multiple theoretical frameworks including the aforementioned χEFT (e.g. [34, 35]) as well as pionless EFT (e.g. [36, 37]), where all pions are integrated out. In this Thesis, χEFT, along with the Valence-Space
In-Medium Similarity Renormalization Group (VS-IMSRG) many-body method discussed in Chapter 3, will be tested against experimental data to establish a baseline.

2.1 The Nuclear Shell Model

The leading model for describing nuclear structure is known as the nuclear shell model due to its similarity to the atomic shell model [12]. Analogously to how the atomic shell model has electrons filling discrete energy shells, both the proton and neutron also fill discrete energy shells in the nucleus. Each of the proton and neutron has a separate set of shells.

2.1.1 Motivation for the Nuclear Shell Model

The existence of discrete energy shells in the nucleus can be seen experimentally by comparing measured binding energies to the liquid drop model (LDM). The LDM treats the nucleus as an incompressible sphere, and predicts bulk properties of the nucleus [12]. This model calculates the binding energy of a given nucleus based on the semi-empirical mass formula

$$B(A, Z) = a_v A - a_s A^{2/3} - a_c \frac{Z(Z-1)}{A} - a_a \frac{(A-2Z)^2}{A} + a_p \frac{\delta A^{1/2}}{A},$$  \hspace{1cm} (2.1)

where $A$ and $Z$ are the number of nucleons and protons respectively, $a_v$, $a_s$, $a_c$, $a_a$, and $a_p$ are volume, surface, coulomb, asymmetry, and pairing constants respectively, and

$$\delta = \begin{cases} 
+1, & \text{even } Z, \text{ even } N \\
0, & \text{odd } A \\
-1, & \text{odd } Z, \text{ odd } N.
\end{cases}$$ \hspace{1cm} (2.2)

These constants are fit to experimental data [12]. By calculating binding energies using the semi-empirical mass formula and subtracting the experimentally measured binding energies, Figure 2.1 can be produced. As both the residuals as a function of proton and neutron are centred around zero, it is clear that the bulk properties of the nucleus are reproduced by the liquid drop model. However, there are significant peaks in both sets of residuals, and these peaks are indicative of nucleon shells. That the peaks arise at the same numbers for both protons and neutrons implies that protons and neutrons are treated similarly in the nuclear
shell model.

Figure 2.1: Binding energy differences between the liquid drop model prediction and experiment as a function of (top) number of protons and (bottom) number of neutrons. Observed magic numbers shown with dashed lines.

2.1.2 The Nuclear Potential

As discussed in [12, 38], the nuclear potential has been experimentally measured to approximately follow the same form as both the nuclear charge radius and the nuclear matter radius. This naturally leads to a starting point known as the Woods Saxon (WS) potential, originally proposed by Woods and Saxon in 1954 [39]. The Woods Saxon potential has the mathematical form

\[
V(r) = \frac{-V_0}{1 + e^{r/R - a}}.
\]  

(2.3)

where \(V_0\) is the potential depth, \(r\) is the distance from the centre of the nucleus, \(R\) is the nuclear radius where \(R = r_0 A^{1/3}\), and \(a\) is the surface thickness, or diffuseness, of the nucleus. An example of this potential is shown in Figure 2.2.
Figure 2.2: A Woods Saxon potential calculated for $A = 74$ using parameter values of $V_0 = 50$ and $a = 0.5$ fm from Eq. 2.3.

The WS potential is used as a mean field potential to calculate nuclear observables in phenomenological methods by fitting experimental data to this form of the potential. However, this method is not used for \textit{ab initio} theoretical methods as the goal of these \textit{ab initio} methods is to create a mathematically consistent model for nuclei without fitting.

2.1.3 Nuclear Shells

After the development of a nuclear potential, this potential can be added to the free space Hamiltonian and applied to the Schrödinger Equation to determine quantized energy states. Using this potential, along with the $2(2\ell+1)$ degeneracy (the $(2\ell+1)$ comes from the $m_\ell$ degeneracy and the additional 2 comes from the $m_s$ degeneracy), energy splittings arise which match experiment relatively well [12]. Shells from the WS potential are shown in Figure 2.3 on the left. The right side of Figure 2.3 shows the WS nucleon shells with the addition of $\ell \cdot s$ splitting, which arises due to the potential difference between aligned and anti-aligned spin-orbit coupling [12].
Though there is degeneracy in the shells already, there is further degeneracy in the nucleus due to the difference between the nucleons. While both protons and neutrons are Fermions and must obey the Pauli exclusion principle, they are different particles and therefore the 0s shell can house two neutrons and two protons. Essentially, each nucleon gets their own set of energy shells.

Figure 2.3: Schematic of energy levels created from the Woods Saxon potential both without (left) and with (right) the effects of spin-orbit coupling. Principle quantum number is one less than the indicated value as here it is labelled as the $n^{th}$ shell with a given $\ell$. Figure taken from [12].
The shells shown in Figure 2.3 on the right are the ones used to describe experimental results [40]. Moreover, it is this potential, with the $\ell \cdot s$ splitting which reproduces the shell closures as expected from experimental observations.

Another potential which can be applied is the 3D Simple Harmonic Oscillator (SHO), and this is the one used for \emph{ab initio} methods [41]. Figure 2.4 shows the shell splittings that appear using the simple harmonic oscillator potential.

\begin{align*}
3s, 2d, 1g, 0i & \quad 168 \quad 2+10+18+26 \\
2p, 1f, 0h & \quad 112 \quad 6+14+22 \\
2s, 1d, 0g & \quad 70 \quad 2+10+18 \\
1p, 0f & \quad 40 \quad 6+14 \\
1s, 0d & \quad 20 \quad 2+10 \\
0p & \quad 8 \quad 6 \\
0s & \quad 2 \quad 2
\end{align*}

Figure 2.4: Schematic of energy level splittings created from simple harmonic oscillator potential. The label on the left are the $\ell$ values included in the shell. The label on the right is the occupancy, split by the $\ell$ in which the occupancies exist. The label in the centre is the total occupancy after that shell. Figure adapted from [12].

Energy shells are labelled by the $\ell$ values within, so the lowest shell is called the $s$ shell and the second is the $p$ shell. These labels can be extrapolated for all shells in Figure 2.4. Shells of interest for this Thesis are the $p$, $sd$ and $fp$ shells as they include the mass range of interest, at least around the $N = Z$ line.

### 2.1.4 Open and Closed Shells

Though nuclear shells can be modelled using different potentials, they all produce distinct energy gaps at what are known as shell closures. These shell closures are where an energy shell is significantly separated in energy from its nearest neighbour, creating a barrier for
nucleons to be excited into a higher-lying shell. This energy barrier is great enough that the typical energy of nucleon-nucleon collisions inside a shell is not great enough to transfer nucleons to the next shell [12].

Due to the Pauli exclusion principle, there are a limited number of possible states a nucleon can occupy within a given shell. As such, in each shell, each possible state is either filled with a nucleon (particle), or empty (hole). If the number of holes in a shell is zero, then the shell is considered to be closed, while if there are a non-zero number of holes then it is an open shell. This is shown schematically in Figure 2.5, where $^{16}\text{O}$ and $^{15}\text{O}$ are used to illustrate open and closed shells created from the WS potential.

![Figure 2.5: Shell depiction of $^{15}\text{O}$ (right) with an open neutron shell and $^{16}\text{O}$ (left) with a completely closed shell core](image)

In Figure 2.5, $^{16}\text{O}$ on the left contains two closed shells, one of protons and one of neutrons, while $^{15}\text{O}$ on the right has an open neutron shell. Due to the open neutron shell in $^{15}\text{O}$, shell model predictions would indicate that the binding of this nucleus would be less than that of $^{16}\text{O}$, which contains a fully closed core [12].

### 2.2 Chiral Effective Field Theory

As mentioned above, the ab initio interactions used in this Thesis fall under the framework of $\chi$EFT, a subset of theoretical methods which aim to calculate nuclear properties from first principles. Though $\chi$EFT has been in use since around the 1990s [33], it is still a prominent focus of theoretical nuclear physics research [42]. Recent advancements in many body methods [33, 43] as well as the increased understanding of the role that $3N$ forces play
[44–46] have allowed $\chi$EFT to calculate nuclear properties into the mid-mass region [47–49] as well as in both open and closed shell systems [50].

2.2.1 The Residual Strong Interaction

QCD has a property called *asymptotic freedom*, meaning that at short length scales (high energy), the coupling is extremely weak and runs to zero. For this reason, though QCD is not always perturbative, the theory can be treated perturbatively at extremely high energy [5]. Inversely, at long length scales (low energy), such as those at the nucleon level, QCD exhibits *confinement* [51], where the coupling constant grows to infinity as the energy decreases. This in turn means that quarks and gluons must exist within bound systems, and cannot be seen as free particles [5]. One possible interpretation of confinement is that the energy required to separate quarks to infinity is greater than the mass-energy of an additional pair of quarks. While this idea was derived from perturbation theory and therefore is not necessarily accurate, it is suggestive of how confinement may work.

Because using QCD introduces quarks and gluons as degrees of freedom, theoretical nuclear physics uses EFTs. This eliminates these irrelevant degrees of freedom and replaces them with the more relevant nucleons and pions. These methods still capture microscopic properties of nuclei without the limitations induced by using quarks and gluons [52]. Interestingly enough, it was the Yukawa’s pion model, introduced roughly 30 years before the quark model of Gell-Mann and Zweig [53], which, with the addition of broken chiral symmetry by Weinberg [54, 55], became what is used today. This model breaks chiral symmetry, a symmetry that if perfect would result in massless pions, both spontaneously (non-zero quark antiquark pairs in the vacuum expectation value) and explicitly (non-zero quark mass). $\chi$EFT is an effective field theory derived by assuming perfect chiral symmetry, and then including chiral symmetry breaking terms such as the non-zero quark mass [56]. In $\chi$EFT, the degrees of freedom are nucleons, the matter fermions, and pions, which are quark antiquark pairs and act as the mediator bosons.
2.2.2 Momentum Cutoffs

While the elimination of degrees of freedom expands the use of the model significantly, the main advantage of $\chi$EFT is that it allows an order-by-order expansion of the nuclear potential, suppressed by powers of a momentum cutoff. This expansion is not a perturbative expansion, but does give reasonable confidence that higher order terms will be of lower magnitude than the lower order terms [52]. The momentum cutoff becomes important as $\chi$EFT is not applicable at high momenta as additional degrees of freedom, such as the substructure of the nucleons and pions, becomes resolved. By separating low and high momenta using this cutoff, the lowest order Lagrangian must include at least two terms, shown schematically in Figure 2.6. More information on $\chi$EFT can be found in [57].

The rate at which successive terms converge is related to the momentum cutoff applied as the expansion is done in terms of the inverse this constant (i.e. the higher the cutoff, the quicker the convergence). While the convergence of order-by-order terms in the expansion becomes quicker with a higher momentum cutoff, the risk of running into the resolution of higher momentum degrees of freedom becomes increasingly relevant. Additionally, there is a characteristic breakdown scale of the momentum cutoff where $\chi$EFT is no longer able to be applied.

\[\text{Figure 2.6: Feynman diagram of one pion exchange plus contact.}\]

Doing this rewriting, the high momentum interactions are captured by the contact term while the low momentum interactions are captured by the pion exchange term. Figure 2.6 does not capture the actual Feynman diagrams used for this Thesis, but schematically shows how a single pion exchange becomes multiple terms: long range pion exchange terms and short range contact terms.
2.3 The Isobaric Multiplet Mass Equation

The first step in the development of theoretical techniques is to ensure that they are able to accurately replicate experimental data that already exists. These benchmark tests must be done for directly calculated values such as binding energies as well as more stringent tests such as differences in the calculated properties between members IAS. In order to test these differences, the *isobaric multiplet mass equation* (IMME) can be used. The IMME is a quadratic equation whose coefficients are sensitive to the Coulomb interaction, non-Coulomb ISB effects, and other subtle differences in binding [42]. Calculating the IMME coefficients using calculated nuclear binding energies from different *ab initio* methods will allow different factors in the theoretical techniques to be tested.

More specifically, the IMME is useful for the purposes of this Thesis because it allows ISB to be studied systematically. This can be done as members of the IATs used for calculation of the IMME coefficients are connected via the isospin ladder operator, $\hat{T}^\pm$, if an assumption of perfect isospin symmetry is made. This means that any deviation from a transition with this operator implies ISB in the decay operator or explicit ISB in the nuclear wavefunctions. Having this property allows the IMME to be a useful tool in studying ISB in nuclei, and an important step in ensuring that *ab initio* methods can be used for the calculation of the ISB correction, $\delta_C$.

2.3.1 Development of the IMME

The IMME (Eq. 2.4) is a quadratic equation relating mass excesses for a set of IAS as a function of three constants and the total isospin projection. The equation was originally proposed by Wigner in 1957 [58], and Weinberg and Treiman in 1959 [59], and is motivated using a first order perturbative expansion of the Coulomb potential in the isospin formalism (See Appendix B for details).

$$M(\alpha, T, T_z) = a(\alpha, T) + b(\alpha, T)T_z + c(\alpha, T)T_z^2$$  \hspace{1cm} (2.4)
Although the IMME is motivated by a first order perturbative expansion of the Coulomb interaction, it has been shown experimentally to be extremely accurate at describing the relationships between mass excesses in larger sets of IAS where the fit is not perfect (e.g. [60, 61]). Even further, it has been shown to accurately predict mass excesses in IAS which are not complete (e.g. [61, 62]), which can have significant impacts in nuclear astrophysics, and more specifically in explaining the physics behind the rapid proton capture process [62, 63]. Incredibly, the ability to use the IMME to predict masses has allowed physicists to set an upper limit on the scalar contribution to the weak interaction [64], but is also accompanied by the ability to predict level energies of certain excited nuclear states [65].

Testing of the IMME has been extensive over the past twenty years, and in general experimental results seem to give good agreement with the IMME (e.g. [60, 65, 66]). However, despite this agreement there is work being done on increasing the number of terms in the IMME (e.g. [61, 67]) in an attempt to include non-negligible strong interaction terms [68–71]. Recently, deviations from the quadratic IMME have been found and the physical explanation for these terms is an active area of research (e.g. [72–77]). However, extending to a $d(\alpha, T)T_z^3$ or higher terms requires more than a triplet for fitting, as there cannot be more fitting parameters than members of the triplet, as well as the limitations placed on the rank of tensors by using $T = 1$ systems.

2.3.2 The IMME Coefficients

The $b$ coefficient in the IMME is the linear term, and for an IAT can be calculated as

$$b = \frac{1}{2} [M(T_z = 1) - M(T_z = -1)], \quad (2.5)$$

which is just half the difference in mass excesses between the two $T_z \neq 0$ terms. The simplicity of Eq. 2.5 comes from the three degrees of freedom in the quadratic IMME and the three terms being fit. Because the $b$ coefficient is determined only from the $T_z = 1$ and $-1$ mass excesses, the value of the term has been attributed to 2-body Coulomb forces between protons [78]. In Towner and Hardy’s phenomenological calculations, the strength
of the 2-body Coulomb force is tuned to match the IMME $b$ coefficient [26]. While the $b$
coefficient does rely heavily on the Coulomb interaction, a uniformly charged sphere does
not perfectly reproduce $b$ coefficients [78], and so it is theorized that anti-symmetrization
terms play a role in the $b$ coefficient as well [79, 80].

The $c$ coefficient, the quadratic term in the IMME, can be calculated exactly as

$$c = \frac{1}{2} \left[ M(T_z = 1) + M(T_z = -1) - 2M(T_z = 0) \right],$$

(2.6)

again because there are three parameters and three members of the IAT. The physics behind
the $c$ coefficient has been attributed to the difference in the relative strengths of the proton-
proton ($pp$) interactions compared to the neutron-neutron ($nn$) interactions, where the $pp$
interactions are roughly 2% stronger than the $nn$ [24, 81, 82]. Towner and Hardy use this
difference to tune their phenomenological calculations to the IMME [26].
CHAPTER 3
VALENCE-SPACE IN-MEDIUM SIMILARITY RENORMALIZATION GROUP

The nuclear potential, created using $\chi$EFT for the purposes of this Thesis, includes low momentum terms coupled to high momentum terms. As the coupling between low and high momentum terms in the potential can cause problems with convergence [52, 83], these can be explicitly decoupled using unitary transformations. These unitary transformations allow $ab\ initio$ calculations of nuclear observables without the convergence problems caused by the low to high momentum coupling [47, 48].

While there are multiple many-body methods, coupled cluster (e.g. [84, 85]), no core shell model (e.g. [86, 87]), self-consistent Green functions (e.g. [88, 89]), and more, the method of interest for this Thesis is the Valence-Space In-Medium Similarity Renormalization Group (VS-IMSRG). This method provides a unitary transformation of the nuclear Hamiltonian to a form which is block diagonal, allowing for a less computationally intensive calculation of nuclear observables including both closed and open shell nuclear binding energies as well as energies of excited states [50].

3.1 Similarity Renormalization Group

The root of VS-IMSRG is the Similarity Renormalization Group (SRG). The basic principle of the SRG method is simple; using unitary transformations on the Hamiltonian the off-diagonal elements can be suppressed, leaving the matrix representation in a band diagonal form. The idea was first introduced in the mid-1990s independently by Wegner [90] and Glazek and Wilson [91, 92], and has been adapted over the past twenty-five years in order to perform more accurate calculations using the same basic principle on increasingly complex systems (e.g. [48, 49, 93, 94]).

The SRG is a method by which a continuous set of unitary transformations suppress off-diagonal elements and drive the matrix representation to its diagonal form [47]. These
transformations are parameterized by a flow parameter, \( s \), in order to perform the transformation to varying degrees. Specifically, this set of unitary transformations form a group with elements \( U(s) \), and performs a change of basis on an operator as

\[
H(s) = U(s)H(0)U^\dagger(s),
\]

where \( H(s) \) is the Hamiltonian after a transformation by parameter \( s \). Ideally, \( U(s) \) would be perfectly unitary which would lead to a perfect change of basis. As physics is basis and reference frame independent, this change of basis would leave the eigenvalues of the Hamiltonian unchanged, therefore being a faithful representation of the Hamiltonian before it was transformed.

Under the SRG method, the Hamiltonian is first split into its diagonal and off-diagonal elements

\[
H(s) \equiv H_d(s) + H_{od}(s),
\]

where the subscripts \( d \) and \( od \) represent diagonal and off-diagonal respectively [47]. Diagonal and off-diagonal are used loosely to represent the elements of the matrix which need to remain as contributors after SRG rotation and those which are to be \textit{rotated out} [83]. This allows for the problem of diagonalizing the Hamiltonian to be written as the two limit expressions in Eq. 3.3.

\[
\lim_{s \to \infty} H(s) \to \lim_{s \to \infty} H_d(s) \\
\lim_{s \to \infty} H_{od}(s) \to 0
\]

More specifically, the problem becomes finding the transformation \( U(s) \) such that the two relations in Eq. 3.3 are satisfied.

The SRG method, as the name suggests, consists of a continuous group of transformations which perform the change of basis. Elements of the group can be described fully by a group generator [95], though in general for the SRG method there are different generators which can be used. Specifically, a generator for the transformations is chosen such that \( H_{od} = 0 \)
occurs at a fixed point in the flow, i.e. \( \frac{dH(s)}{ds} = 0 \), which means that if \( H_{od}(s = 7) = 0 \), then running the SRG flow from \( s = 7 \) to \( s \to \infty \) would result in no further significant changes.

In Wegner’s introduction of the SRG method, the generator
\[
\eta(s) = [H_d(s), H(s)] = [H_d(s), H_{od}(s)]
\]
was used [90], which forces the off diagonal element to zero as \( s \to \infty \) [47, 48, 96]. While this generator is effective, another generator, proposed by White in 2002 [97] in a quantum chemistry context, can also be used. This generator has the form
\[
\eta \equiv \frac{H_{od}}{\Delta},
\]
where \( \Delta \) is an energy denominator. For the purposes of this Thesis, a more general form of this generator is used, following the mathematical form
\[
\eta \equiv \frac{1}{2} \arctan \left( \frac{2H_{od}}{\Delta} \right),
\]
which for small arguments of the arctan results in Eq. 3.5. More information on this generator can be found in [97].

Implementation of the generator in the SRG framework is done by taking the derivative of the transformation (Eq. 3.1) with respect to the flow parameter \( s \)
\[
\frac{dH(s)}{ds} = \frac{dU(s)}{ds} H(0) U^\dagger(s) + U(s) H(0) \frac{dU^\dagger(s)}{ds},
\]
strategically multiplying by the identity
\[
\frac{dH(s)}{ds} = \frac{dU(s)}{ds} \left( U^\dagger(s) U(s) \right) H(0) U^\dagger(s) + U(s) H(0) \left( U^\dagger(s) U(s) \right) \frac{dU^\dagger(s)}{ds},
\]
and simplifying the expression
\[
\frac{dH(s)}{ds} = \frac{dU(s)}{ds} U^\dagger(s) H(s) + H(s) U(s) \frac{dU^\dagger(s)}{ds}.
\]
By defining the generator
\[ \eta(s) \equiv \frac{dU(s)}{ds} U^\dagger(s) = -\eta^\dagger(s), \] (3.10)
the differential equation written in Eq. 3.9 can be written as the SRG flow equation for the Hamiltonian (Eq. 3.11)
\[ \frac{d}{ds} H(s) = [\eta(s), H(s)]. \] (3.11)

An example of the implementation of this method for the diagonalization of an arbitrary 2×2 matrix can be found in Appendix C. This example uses the White generator defined in Eq. 3.5, and simply illustrates the method being used.

By using the generator of the group rather than the explicit forms of the unitary transformations included in the group, the SRG method can be used more readily as the set of unitary transformations specific to a given Hamiltonian never have to be made explicitly. This allows the SRG method to be used for a variety of nuclei.

The SRG method itself is used in the context of χEFT to soften the potential. By suppressing the off diagonal elements of the potential, high and low momentum interactions are decoupled, the potential is said to be softer, and the diagonalization of the resulting Hamiltonian easier [96].

### 3.2 Valence-Space In-Medium Similarity Renormalization Group

After the SRG method is used to soften the potential, the nuclear Hamiltonian then can be shifted into a different form more specific to the individual nucleus. This process, which is rooted in SRG, is the Valence-Space In-Medium SRG (VS-IMSRG). The VS-IMSRG is a many-body method specifically tailored to a given nucleus [50], and implements the same flow equations as the generic, free space SRG, but does this process in medium rather than in free space. The specifics of VS-IMSRG and the differences between VS-IMSRG and free space SRG require the introduction of normal ordered operators and Wick’s theorem in order to reduce the induced 3N, 4N, and higher-N interactions from the SRG flow [52].
3.2.1 Normal Ordering of Operators

In second quantization, creation and annihilation operators can be classified as Bosonic or Fermionic by their defining commutation relation. Bosonic operators follow a commutation relation defined in Eq. 3.12 as particles obey Bose-Einstein statistics. In contrast, Fermionic operators follow an anti-commutation relation defined in Eq. 3.13 as particles obey Fermi-Dirac statistics.

\[
\left[ a_i, a_j \right] = \left[ a_i^\dagger, a_j^\dagger \right] = 0, \quad \left[ a_i, a_j^\dagger \right] = \delta_{ij} \tag{3.12}
\]

\[
\left[ a_i, a_j \right]_+ = \left[ a_i^\dagger, a_j^\dagger \right]_+ = 0, \quad \left[ a_i, a_j^\dagger \right]_+ = \delta_{ij} \tag{3.13}
\]

As nucleons are Fermions, the nuclear Hamiltonian can be written in terms of Fermionic creation and annihilation operators rather than their Bosonic counterparts. Normal ordering is defined as

\[
\langle 0 \mid \left\{ a_1^\dagger \ldots a_N^\dagger a_N \ldots a_1 \right\} \mid 0 \rangle = 0, \tag{3.14}
\]

where the product of operators in braces (\( \left\{ a_i^\dagger a_j \right\} \)) represents normal ordering. The exact ordering is specific to the state being used for the expectation value, which in this case is the vacuum. One important note to make is that within a normal ordered set of operators, the application of the Fermionic anti-commutation relation can be used freely \[52\], and is implemented as in Eq. 3.15.

\[
\left\{ \ldots a_i^\dagger a_j \ldots \right\} = - \left\{ \ldots a_j a_i^\dagger \ldots \right\} \tag{3.15}
\]

With normal ordering of operators now defined, the difference between the SRG and IMSRG methods can be noted. SRG methods use normal ordering of operators with respect to the vacuum as in Eq. 3.14, but IMSRG does this process in medium, which means rather than using the vacuum as the reference state for normal ordering, the IMSRG method uses a finite density reference state \( | \Psi \rangle \). Mathematically this is equivalent to Eq. 3.16

\[
\langle \Psi \mid \left\{ a_1^\dagger \ldots a_N^\dagger a_N \ldots a_1 \right\} \mid \Psi \rangle = 0, \tag{3.16}
\]
where $|\Psi\rangle$ is the finite density reference state mentioned above. Here, the normal ordering is defined for the specific reference state, in contrast to Eq. 3.14 where the order was defined by the vacuum. By defining $|\Psi\rangle$ to be the ground state of the nearest closed shell [49, 94] the IMSRG process becomes more tailored to the specific nucleus leading to a more accurate calculation of the nuclear Hamiltonian [50].

### 3.2.2 Wick’s Theorem

The implementation of normal ordering of operators, at least for the context of this Thesis, is Wick’s theorem, first introduced in 1950 to help simplify Feynman calculus [98]. Wick’s theorem allows any set of $n$ creation and $n$ annihilation operators to be written in a way which reduces the number of terms that contribute to the expectation value. Specifically, Wick’s theorem lets any set of $n$ creation and $n$ annihilation operators to be written as their normal ordered form added to a recursive sum of their contractions, as shown in Eq. 3.17 for $n = 2$. Wick’s theorem can be extended to any $n$ creation and $m$ annihilation operators [41, 99], but for the purposes of this Thesis will only be considered for cases where there are $n$ creation and $n$ annihilation operators.

$$
\begin{align*}
    a_i^\dagger a_j^\dagger a_l a_k &= \left\{ a_i^\dagger a_j^\dagger a_l a_k \right\} + \left\{ a_i^\dagger a_j^\dagger a_l a_k \right\} - \left\{ a_i^\dagger a_l a_j^\dagger a_k \right\} - \left\{ a_i^\dagger a_l a_j^\dagger a_k \right\} \\
    &+ \left\{ a_i^\dagger a_k a_j^\dagger a_l \right\} + \left\{ a_i^\dagger a_k a_j^\dagger a_l \right\} - \left\{ a_i^\dagger a_j a_l a_k \right\} \\
    &= \left\{ a_i^\dagger a_j^\dagger a_l a_k \right\} + \left\{ a_i^\dagger a_k a_j^\dagger a_l \right\} + \left\{ a_i^\dagger a_k a_j^\dagger a_l \right\} - \left\{ a_i^\dagger a_l a_j^\dagger a_k \right\} \\
    &- \left\{ a_i^\dagger a_l a_j^\dagger a_k \right\} + \left\{ a_i^\dagger a_k a_l a_j^\dagger \right\} - \left\{ a_i^\dagger a_l a_j^\dagger a_k \right\} \\
    &= \{ a_i^\dagger a_j^\dagger a_k a_l \} + \{ a_i^\dagger a_l a_j^\dagger a_k \} + \{ a_i^\dagger a_l a_j^\dagger a_k \} - \{ a_i^\dagger a_l a_j^\dagger a_k \} \\
    &- \{ a_l a_j a_i^\dagger a_k \} + \{ a_l a_k a_j a_i^\dagger \} - \{ a_l a_k a_j a_i^\dagger \} \\
    &= \{ a_i^\dagger a_j^\dagger a_l a_k \} + \{ a_i^\dagger a_l a_j^\dagger a_k \} + \{ a_i^\dagger a_l a_j^\dagger a_k \} - \{ a_i^\dagger a_l a_j^\dagger a_k \} \\
    &- \{ a_l a_j a_i^\dagger a_k \} + \{ a_l a_k a_j a_i^\dagger \} - \{ a_l a_k a_j a_i^\dagger \} \\
    &- \{ a_l a_j a_i^\dagger a_k \} + \{ a_l a_k a_j a_i^\dagger \} - \{ a_l a_k a_j a_i^\dagger \} \\
    &= \{ a_i^\dagger a_j^\dagger a_l a_k \} + \{ a_i^\dagger a_l a_j^\dagger a_k \} + \{ a_i^\dagger a_l a_j^\dagger a_k \} - \{ a_i^\dagger a_l a_j^\dagger a_k \}
\end{align*}
$$

(3.17)

The contraction between two operators is the expectation value of these operators with respect to the reference state being used for normal ordering [52, 100]. More specifically, the contraction between the $i^{th}$ and $j^{th}$ creation and annihilation operators respectively is just the $ij$ element of the one body density matrix of the reference state $|\Psi\rangle$ [101]

$$
\begin{align*}
    a_i^\dagger a_j &= \langle \Psi | a_i^\dagger a_j | \Psi \rangle = \rho_{ij}.
\end{align*}
$$

(3.18)
Because $\rho_{ij}$ is not an operator, it can be removed from the inner product and treated as a scalar. This allows the contraction to be removed from the set of operators and be multiplied by the remaining, normal ordered operators.

### 3.2.3 Valence Space Decoupling

The end goal of the VS-IMSRG many body method is to take a complicated Hamiltonian and decouple the valence shell in order to solve for nuclear observables in a manner specific to a given nucleus. This method has been shown to, with an appropriate selection of reference states for the normal ordering of operators, reproduce accurately both closed and open shell binding energies as well as energies of excited states [50]. This is because by transforming the Hamiltonian into a block diagonal form where all relevant information is contained in one block, the resulting Hamiltonian becomes easier to diagonalize and reduces the computational cost of diagonalization [83].

In order for a single block in the block diagonal form of the Hamiltonian to contain all relevant information, a change of basis first needs to be done from a potential style basis, such as a plane wave or momentum basis, to a basis with $n$ particle, $n$ hole transitions, such as the harmonic oscillator basis. More specifically, the Hamiltonian is transformed using a Fock-space representation of all possible states in the harmonic oscillator basis, such that, when transformed to a block diagonal form, blocks exist for the “valence” and “not valence” spaces.

The *valence space* part of the VS-IMSRG corresponds to how the matrix representation of the Hamiltonian is then treated; different shells in the nucleus are decoupled from one another through the implementation of the flow equations. This occurs because the transformation suppresses terms in the interactions which cause excitations between shells. This is shown schematically in Figure 3.1.

Though Figure 3.1 is a schematic, and the energy spacing between the different shells is not shown to scale and does not need to be consistent between protons and neutrons even for the same shell, it does depict how the valence space decoupling works. By performing this
decoupling the closed shell cores can be diagonalized (though there is only one configuration) and the valence space can be diagonalized separately. The higher lying shells are decoupled and not included in any diagonalization.

### 3.3 Summary of VS-IMSRG

In order to begin using the VS-IMSRG many-body method, the first step is creating the potential using $\chi$EFT, which is typically done in momentum space. Figure 3.2(a) shows a possible potential created in this manner where the two axes are momenta of nucleons, and each block in Figure 3.2(a) is a matrix element. In this matrix representation, elements along the diagonal couple similar momenta between the nucleons and far from the diagonal couple high and low momenta together. Initially, in taking the Feynman diagrams used in $\chi$EFT, there is no SRG softening, and these elements can have non-negligible magnitudes.

In Figure 3.2(a), darker colours represent interaction matrix elements with greater magnitude, while white matrix elements are zero. The potential shown is simply a schematic potential and is not necessarily representative of a realistic potential created using $\chi$EFT.
Figure 3.2: Schematic representations of matrices derived using $\chi$EFT for (a) generated potential and (b) after SRG softening. Darker colours indicate elements with higher magnitudes.

Because coupling between high and low momentum interactions causes issues with convergence, they are often rotated out using the SRG methods, resulting in softer interactions. In order to do this rotation, the SRG flow equation (Eq. 3.11) can be run forward step by step until the potential is softened effectively. Though softer interactions produce more well behaved interactions with better convergence [102], the further the SRG evolution is taken, the greater the SRG error becomes as the size of the resulting matrix decreases [103]. This size is not the rank of the matrix, but rather the width of the remaining band in the band diagonal form produced. The width of the band is denoted with an SRG scale, where larger cutoffs indicate wider bands and a harder interaction. This cutoff is independent from the $\chi$EFT interaction itself, and the specific SRG cutoff being used is reported with the interaction when being used for calculations.

The resulting matrix from the SRG flow has a band diagonal structure, shown schematically in Figure 3.2(b), where the same colouring scheme as Figure 3.2(a) is used. The matrix representations in Figure 3.2(a) and Figure 3.2(b) are in the same style of basis, though
they must be in different bases as an SRG rotation was performed. It can be seen that by performing the SRG evolution, the off diagonal elements of the potential are suppressed. This results in the decoupling of high momentum and low momentum interactions, which was the goal of the SRG method at the outset. Figure 3.2(b), while schematically showing the result of SRG flow, is not completely indicative of the resulting matrix, as it is an idealized model. In reality, the suppression is not always perfect, leaving non-negligible matrix elements in the off diagonals, and the diagonal elements are not all of the same magnitude. The general shape of the matrix shown in Figure 3.2(b) is generally indicative of the result of SRG softening.

The SRG softened potential schematically shown in Figure 3.2(b) is what is fed into the VS-IMSRG method, which is used to decouple energy levels. In order for this to be done, the SRG softened potential needs to be changed from the potential style basis into a particle-hole basis, such as the harmonic oscillator basis. Because the actual harmonic oscillator basis is infinite, with shells extending \textit{ad infinitum} beyond those shown in Figure 2.4, the basis needs to be truncated for any finite calculations to be done. This truncation is done using a parameter called $e_{\text{max}}$, which scales with the harmonic oscillator shells as $e_{\text{max}} = \max(2n+\ell)$. For example, $e_{\text{max}} = 2$ would allow the basis to include the $s$ shell $(2(0)+0=0)$, the $p$-shell $(2(0)+1=1)$, and the $sd$-shell $(2(1)+0=2(0)+2=2)$, but would not allow the $fp$-shell $(2(1)+1=2(0)+3=3>2)$ to be included in the basis. In this basis, the matrix form of the Hamiltonian derived using $\chi$EFT will increase factorially with $e_{\text{max}}$, making higher $e_{\text{max}}$ calculation more computationally expensive. The exact dimension of the Hamiltonian can be calculated as in Eq. 3.19

$$\text{rank} = \left( \sum_{i=0}^{e_{\text{max}}} n_i \right) \left( \sum_{i=0}^{e_{\text{max}}} n_i \right) \quad (3.19)$$

where $i$ is a placeholder for the shells in Figure 2.4 (i.e. $i = 0$ represents the $s$ shell), $n_i$ represents the number of particles possible in the $i^{th}$ shell, $N$ is the number of neutrons, and
$Z$ is the number of protons. The sum in Eq. 3.19 can be simplified as

$$
\sum_{i=0}^{e_{\text{max}}} n_i = \frac{1}{3}(e_{\text{max}} + 1)(e_{\text{max}} + 2)(e_{\text{max}} + 3).
$$

As $e_{\text{max}}$ is increased and the truncation lessened, it is expected that the resulting calculations will converge as the effect of the higher shells become negligible due to energy considerations. Because of this, once the results have converged they will not likely vary much at any higher $e_{\text{max}}$.

After switching to this basis, truncated by $e_{\text{max}}$, the potential is transformed into a block diagonal form using the IMSRG flow equations. These equations are written in Eqs. 3.21, 3.22, and 3.23 for the zero body, one body, and two body forces respectively [52]. By flowing these three coupled differential equations forward with parameter $s$ and using an appropriate normal ordering reference state and the White generator, the block diagonal form shown in Figure 3.3 can be produced, effectively decoupling the states of interest.

$$
\frac{dE}{ds} = \sum_{ab} (n_a - n_b) \eta_{ab} f_{ba} + \frac{1}{2} \sum_{abcd} \eta_{abcd} \Gamma_{cdab} n_a n_b \overline{n}_c \overline{n}_d
$$

$$
\frac{df_{ij}}{ds} = \sum_a (1 + P_{ij}) \eta_{ia} f_{aj} + \sum_{ab} (n_a - n_b)(\eta_{ab} \Gamma_{biaj} - f_{ab} \eta_{biaj})
+ \frac{1}{2} \sum_{abc} (n_a n_b \overline{n}_c + \overline{n}_a n_b n_c)(1 + P_{ij}) \eta_{ciab} \Gamma_{abcj}
$$

$$
\frac{d\Gamma_{ijkl}}{ds} = \sum_a \{(1 - P_{ij})(\eta_{ia} \Gamma_{ajkl} - f_{ia} \eta_{ajkl}) - (1 - P_{kl})(\eta_{ak} \Gamma_{ijal} - f_{ak} \eta_{ijal})\}
+ \frac{1}{2} \sum_{ab} (1 - n_a - n_b)(\eta_{jab} \Gamma_{abkl} - \Gamma_{ijab} \eta_{abkl})
+ \sum_{ab} (n_a - n_b)(1 - P_{ij})(1 - P_{kl}) \eta_{abk} \Gamma_{bjal}
$$

In Eqs. 3.21, 3.22, and 3.23 these equations $n_a$ represents the particle occupancy number for the $a$th state (i.e. if the state is filled $n_a = 1$ otherwise $n_a = 0$), and $\overline{n}_a$ represents the inverse of this (i.e. $\overline{n}_a = 1 - n_a$), and are specific to the reference state used. The $f_{ij}$ and $\Gamma_{ijkl}$ terms represent matrix elements from the $\chi$EFT interaction potential. Finally, the
$P_{ij}$ represents the permutation of the terms under the $i$ and $j$ indices. These terms simply capture terms in the differential equations with the same form but an exchange of indices.

Figure 3.3: Block diagonal schematic form of matrix representation of nuclear potential after VS-IMSRG flow. The labels $P$ and $Q$ represent the space of interest and the higher energy shells respectively.

In Figure 3.3, the Hamiltonian is split into the region of interest ($P$), and the regions of non-interest ($Q$), based on the harmonic oscillator shells accessible to nucleons. By doing this, the elements of the $P$ region can be diagonalized while ignoring the effects on the $Q$ regions, reducing computation time and increasing efficiency. As with Figure 3.2(a) and Figure 3.2(b), Figure 3.3 is not a perfect representation of the form that the matrix representation of the Hamiltonian will take but is a good schematic representation. Likewise, the elements in each region do not have to be identical to each other and can vary.

The final diagonalization is done for only the $P$ region, or the region of interest, though this matrix is never explicitly constructed. This makes the final diagonalization much less computationally expensive and allows for an exact diagonalization of the space of interest.
CHAPTER 4
CALCULATION METHOD

The purpose of this Chapter is to outline the connection between the $\chi$EFT interactions used and the final output of binding energies used for the calculation of the IMME. This Chapter will give a procedure for the work completed including which $\chi$EFT interactions are used as inputs to the VS-IMSRG many-body method through the diagonalization of the $P$ block produced.

4.1 The $\chi$EFT Interactions Used

The first $\chi$EFT interaction being used in this Thesis is the EM1.8/2.0 interaction discussed in detail in [104]. The base of this interaction is the next-to-next-to-next-to leading order (N3LO) $NN$ forces at a 500 MeV momentum cutoff developed by Entem and Machleidt [105], and are combined with N2LO 3$N$ forces from [106, 107], cutoff at 2.0 fm$^{-1}$ ($\approx 400$ MeV). The $NN$ part of the potential created from these forces is SRG softened to 1.8 fm$^{-1}$ ($\approx 350$ MeV). Low energy constants for this interaction were fit to the $^3$H binding energy and the $^4$He matter radius [108, 109]. The EM1.8/2.0 interaction has been shown to reproduce nuclear binding energies accurately (e.g. [42, 110, 111]), though slightly overbound in the $sd$-shell. Additionally, there has been some evidence that the excitation energies calculated using this interaction are slightly too high [104].

In addition to the EM1.8/2.0 interaction, a second interaction is used in this Thesis and is labelled N2LOsat, which uses N2LO for both $NN$ and 3$N$ forces with no SRG softening [112]. These forces are computed with a momentum cutoff of 450 MeV. This interaction uses both $NN$ and 3$N$ forces when fitting the low energy constants [112], in contrast with EM1.8/2.0 which only uses $NN$ forces. While N2LOsat does not predict ground state binding energies as well as EM1.8/2.0 [104, 113], it has been shown to accurately reproduce nuclear
charge radii [112], an important consideration in the modeling of Coulomb repulsion between protons.

The N2LOsat interaction is harder than the EM1.8/2.0 interaction in that the N2LOsat interaction is not SRG softened at any scale while the EM1.8/2.0 interaction is. With no SRG softening, there is no decoupling between the high and low momentum degrees of freedom in the interaction, though there is still a cutoff. This should result in a significantly slower convergence with increasing $e_{\text{max}}$ for N2LOsat when compared to EM1.8/2.0.

In this Thesis, the resulting matrices from these interactions are never explicitly seen but the matrix elements from the potentials (with the EM1.8/2.0 interaction SRG softened) used as an input to the VS-IMSRG many-body method.

### 4.2 VS-IMSRG Many-Body Method Code

Implementation of the VS-IMSRG many-body method was done using a revised version of the IMSRG code developed by Stroberg et al [114], which employs the *magnus* formulation of IMSRG [115]. This formulation results in first-order Euler methods being possible for solving the IMSRG flow equations and increases computational efficiency.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>EM1.8/2.0</th>
<th>N2LOsat</th>
</tr>
</thead>
<tbody>
<tr>
<td>file2e1max</td>
<td>14</td>
<td>14</td>
</tr>
<tr>
<td>file2e2max</td>
<td>28</td>
<td>14</td>
</tr>
<tr>
<td>file2lmax</td>
<td>14</td>
<td>14</td>
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<tr>
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</tr>
<tr>
<td>file3e3max</td>
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<tr>
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<td>16</td>
<td>14</td>
</tr>
<tr>
<td>hw</td>
<td>16</td>
<td>20</td>
</tr>
<tr>
<td>$A,Z,e_{\text{max}},\text{VS}$</td>
<td>Case</td>
<td>Case</td>
</tr>
</tbody>
</table>

Parameters specified in the IMSRG code are listed in Table 4.1, with some specified differently for the two interactions. The first six parameters listed in Table 4.1 indicate
maximum values for the $NN$ and $3N$ interaction files. These need to be specified because the interaction files are simply a list of numbers representing matrix elements, and without these parameters the IMSRG code could not interpret the matrix elements correctly [83]. The parameter ‘e3max’ specifies the $e_{\text{max}}$ truncation used for the $3N$ forces only, and is set to be the largest possible value given the parameters of the matrix elements. The ‘hw’ parameter is the harmonic oscillator frequency for the potential, $\hbar \omega$. $A$, $Z$, $e_{\text{max}}$, and the valence space (VS) are specified on a case by case basis, and are used as inputs to the IMSRG method rather than static parameters.

After these parameters were set for the interactions, the code was adjusted to reduce memory usage by writing unnecessary output to ‘/dev/null/’. While this output is required for the transformation of operators under SRG rotations [28], it is not required for binding energy calculations [83]. This adjustment was made to allow the calculations of binding energies to be done more efficiently both in computation time and memory use.

The IMSRG code was also adjusted to take terminal inputs for $A$, $Z$, $e_{\text{max}}$, and the valence space decoupling scheme. In adding this functionality, because $Z$ and $e_{\text{max}}$ were set up to allow a list of values, some of the list structure in the IMSRG code had to be changed. By introducing terminal inputs for these often-adjusted parameters, the IMSRG code could then be run without editing the file each time. Specifically, this allowed the IMSRG code to be run from either the command line or another script, increasing overall calculation efficiency by introducing the ability to perform sequential steps from a wrapper. This wrapper is discussed in detail in Section 4.4.

Outputs from the IMSRG code included two files of interest, an interaction (‘.int’) and a model space (‘.sp’) file. Both of these files are required as inputs to the shell model diagonalization, discussed in Section 4.3. Also included in the interaction file is the binding energy of the core shells decoupled from the valence space. This binding energy is simply a $1 \times 1$ matrix as there is only one possible configuration of particles in a completely closed core.
4.3 Shell Model Diagonalization

Diagonalization and calculation of the valence space binding was done using NuShellX@MSU [116]. This requires the input of an interaction file and a model space file, which are produced by the IMSRG code. NuShellX@MSU takes these input files and uses a \( J \)-coupled basis for protons and neutrons to produce exact eigenvalues.

Additionally, NuShellX@MSU requires knowledge of various parameters specific to the nucleus in question in order to calculate the eigenvalues, and these need to be input before the diagonalization takes place. Parameters input into NuShellX@MSU are listed in Table 4.2.

Table 4.2: Parameters used in the NuShellX@MSU code for exact calculation of eigenvalues for the valence space

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Input</th>
</tr>
</thead>
<tbody>
<tr>
<td>Option</td>
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</tr>
<tr>
<td>Model Space</td>
<td>.sp file from IMSRG</td>
</tr>
<tr>
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<td>n (no)</td>
</tr>
<tr>
<td>Interaction</td>
<td>.int file from IMSRG</td>
</tr>
<tr>
<td>Number of Protons</td>
<td>( Z )</td>
</tr>
<tr>
<td>Number of Nucleons</td>
<td>( A )</td>
</tr>
<tr>
<td>( \text{minJ,maxJ,delJ} )</td>
<td>( 0,1,1 )</td>
</tr>
<tr>
<td>Parity ( (0 \text{ for } +, 1 \text{ for } -, 2 \text{ for both}) )</td>
<td>( 2 )</td>
</tr>
</tbody>
</table>

The ‘Option’ parameter accounts for the calculation to be done. NuShellX@MSU can calculate both wavefunctions and overlap of wavefunctions, and the ‘lpe’ input tells NuShellX@MSU to calculate wavefunctions. The ‘Restrictions’ parameter allows for the truncation of model space or other restrictions to be put on the calculation, but were never used in this Thesis. The \( J \) and ‘Parity’ parameters tells NuShellX@MSU which spin-parity states to calculate, and were selected to ensure that there were enough states calculated to include the lowest \( 0^+ \) state without calculating too many states and making the calculation take longer.
4.4 Implementation of VS-IMSRG and NuShellX@MSU

Both the VS-IMSRG and NuShellX@MSU codes are run through a wrapper, the entirety of which is shown in Appendix D. This wrapper, which was a significant portion of code development in this Thesis, allows for a significantly more efficient systematic study of the \textit{ab initio} methods used. This is because sequential steps, from the implementation of the VS-IMSRG through the shell model diagonalization.

Inputs into the wrapper are taken from the command line with the command

\begin{verbatim}
python RunThis.py A Z e VS,
\end{verbatim}

where $A$, $Z$, $e$, and $VS$ are input parameters for the mass number, number of protons, $e_{\text{max}}$, and valence space decoupling scheme used. Both $e_{\text{max}}$ and $Z$ can take multiple inputs as a string, which are split into a list in the IMSRG code. These parameters are then passed into the IMSRG code. The output files from which, including the interaction and model space files, are saved to disk at the end of the IMSRG rotation.

Because the IMSRG code is written in such a way as to accept multiple arguments for $e_{\text{max}}$ and $Z$ and output files for the IMSRG are created for all, the inputs are split into lists and looped through for the rest of the process. The NuShellX@MSU, when run, creates numerous files and therefore a new directory was made for each nucleus at each $e_{\text{max}}$. After copying the output files from the IMSRG code to this new directory, the files were renamed in order to run NuShellX@MSU the same for each case.

Running NuShellX@MSU requires parameters specific to the nucleus as shown in Table 4.2, and therefore a file was created which can be called when performing the calculation of eigenvalues rather than having to input them all sequentially. The output of NuShellX@MSU includes a single file with the level energies for the states calculated.

The final step in the process is to take the zero-body energy of the bound state contained in the interaction file from the IMSRG rotation and adding it to the energy calculated by NuShellX@MSU for the valence space, and saving this to file to be read later for analysis.
CHAPTER 5
BENCHMARKING THEORETICAL METHODS USING THE IMME

As discussed in Section 2.3, before a theoretical technique can be used to perform tests of the SM, it first needs to be tested against known experimental results. Unfortunately, as $\delta_C$ cannot be measured experimentally, these results need to come from other sources which are sensitive to ISB in the nuclear potential. One method for doing this is by comparing \textit{ab initio} calculations of the IMME coefficients against experimental results. The purpose of this section is exactly that; to study the IMME coefficients calculated using the \textit{ab initio} methods against those measured experimentally with the hope of understanding sources of ISB in the nuclear potential and guiding further theoretical efforts.

5.1 Isobaric Analogue Triplets Studied

In order to perform a systematic test of \textit{ab initio} methods using the IMME, cases were first needed to be identified. For the purposes of this Thesis, the mass range of $A = \{10 : 74\}$ was used, every four (i.e. 10, 14, ..., 70, 74). These were chosen because they represent the relevant superallowed IATs in the $p$, $sd$, and $fp$-shells, of which at least two of the members of the IAT have mass excesses measured precisely [78].

For each of these members, the lowest lying $0^+$ state was used. For most of these cases, including all $|T_z| = 1$ states, this was the ground state. However, for some $N = Z$ nuclei, the ground state did not have 0 spin, in which case the lowest excited $0^+$ state was used. Specific states studied in this Thesis are summarized in Appendix E with their experimental values.

5.2 Convergence of Calculations

The first step in attempting to understand the results of \textit{ab initio} calculations is to ensure that the calculated values accurately reflect the interactions, and to do so, the calculations
must be converged. Specifically, the calculated values must converge with \( e_{max} \), as this is the parameter controlling the number of basis states used to create wavefunctions in the many body method. By running \( e_{max} \to \infty \), the output of the many body method will be indicative of the interactions used. However, as time and computational resources are limited, \( e_{max} \) cannot be run to extremely high values, but as increasing \( e_{max} \) increases the number of basis states used, the higher lying of which do not contribute significantly to the wavefunctions in question, it is expected that once calculations converge with \( e_{max} \) there will be little to no deviation at higher \( e_{max} \) [104].

In order to test convergence, binding energies were calculated for each nucleus, using both interactions, at \( e_{max} = \{6, 8, 10, 12\} \). The selection of \( e_{max} \) values was done such that the first calculation would be computationally inexpensive, and that the calculation will have converged by the time the calculation was done with the final \( e_{max} \). The steps of 2 in \( e_{max} \) allows for HO shells of consistent orbital angular momentum to be added, rather than adding even and odd angular momentum shells every other step in \( e_{max} \).

5.2.1 Mass Excess Convergence

As the ab initio methods calculate binding energies and the IMME is typically done using mass excess [78], a conversion between binding energy and mass excess was needed to be done. Beginning with the binding energy in MeV, which will be a negative value for a bound system, the mass of the nucleus can be found by adding the masses of the composite particles

\[
m = E_B + Zm_H + Nm_n,
\]

where \( m_H \) and \( m_n \) are the masses of a neutral hydrogen atom and the neutron respectively. The mass excess of an atom is then the difference between this mass, converted into atomic mass units (amu), and the number of nucleons in the system.

\[
M = m - (N + Z)
\]
The mass excess in keV or similar units can then be found through a unit conversion back from amu. For the purposes of this Thesis, mass excesses will be reported in keV, and are calculated using this prescription.

![Mass Excess Convergence for A = 34](image)

Figure 5.1: Mass excesses of the $A = 34$ IAT calculated using both EM1.8/2.0 and N2LOsat plotted with experimental values. Solid colored lines represent an exponential extrapolation of the $e_{max} = \{8, 10, 12\}$ points.

Figure 5.1 shows graphically the convergence of mass excesses calculated for $A = 34$. This is seen in the other masses as well, and these plots can be found in Appendix F.

It can be seen that for both interactions the mass excess, and therefore binding energies, converge with increasing $e_{max}$, and that by $e_{max} = 12$, the calculations have converged, or are at least very close and running an exponential fit to the points will have little effect. This can be seen explicitly in the extrapolated values plotted alongside the calculated points, where the calculated point at $e_{max} = 12$ often overlaps with the extrapolation curve. These extrapolated values are calculated using the $e_{max} = \{8, 10, 12\}$ points, as it can be seen visibly that the calculation of $e_{max} = 6$ has not yet included enough basis states to accurately represent the interaction. The extrapolation done was exponential, using

$$M(e_{max}) = Ae^{-Be_{max}} + C,$$

(5.3)
where $A$, $B$, and $C$ and fitting coefficients. As there were three data points used in the fit, the extrapolated value can be calculated analytically.

Also seen in the convergences of mass excess shown in Figure 5.1 and Appendix F is that the EM1.8/2.0 interaction converged faster with $e_{\text{max}}$ than the N2LOsat interaction. This aligns with the relative softness of the interaction and the assertion that the coupling of high and low momentum interactions in the nuclear potential creates issues with convergence.

As noted above, the calculations have converged by $e_{\text{max}} = 12$, and therefore the $e_{\text{max}} = 12$ calculations can then be considered a reliable representation of the interactions used. Due to this level of convergence, it is reasonable to proceed with confidence to calculating the IMME coefficients using these interactions.

### 5.2.2 IMME $b$ Coefficient Convergence

Though there is convergence in the mass excesses calculated, the values to which the ab initio methods approach do not match those of experiment. Looking more closely, the amount by which the mass excesses do not approach experiment seem to be off by a systematic shift. In calculating the IMME coefficients, this systematic shift should be removed, or at least reduced, as there are an equal number of terms being added and subtracted. Having the convergence in mass excess should lead to the IMME coefficients converging systematically with $e_{\text{max}}$ and the systematic shift in calculated mass excesses should lead to more accurate calculations of the coefficients when compared to experiment.

Figure 5.2 shows a typical convergence plot for the $b$ coefficients, and is for $A = 34$. The remainder of these plots are shown in Appendix I.

In Figure 5.2, both curves show exponential convergence; the same trend seen in mass excess convergences. However, unlike the mass excess convergences, the $b$ coefficients did not converge by $e_{\text{max}} = 12$, indicating that the rate of convergence in the mass excesses was not constant between masses. As the $b$ coefficients were not converged by $e_{\text{max}} = 12$, some extrapolation is necessary to accurately represent the interaction. In order to do so, the
Figure 5.2: IMME $b$ coefficient calculated for $A = 34$ as a function of $e_{\text{max}}$ ranging from $e_{\text{max}} = 6$ through $e_{\text{max}} = 12$ in order to check convergence. Solid coloured lines represent an exponential extrapolation of the $e_{\text{max}} = \{8, 10, 12\}$ points.

The same extrapolation as for the mass excesses was applied

$$b(e_{\text{max}}) = Ae^{-Be_{\text{max}}} + C. \quad (5.4)$$

These extrapolated values are shown as solid lines in Figure 5.2, and are what is used for further analysis. It was this extrapolation used rather than the $b$ coefficients calculated using the extrapolation of mass excess because there are correlated errors in the mass excesses. As the $ab$ initio interactions have inherent approximations in them, it is more accurate to extrapolate the $b$ coefficients as many of these are systematic between nuclei.

As with the convergence of mass excesses, it is seen that the EM1.8/2.0 interaction converged faster with $e_{\text{max}}$ than the N2LOsat interaction for the $b$ coefficient. This is likely a direct product of the rate of convergence of the mass excesses, and is still indicative of the effects of SRG softening.

Taking a closer look at Appendix I it is clear that while all masses greater than $A = 10$ appear to converge exponentially, $A = 10$ does not. This is shown clearly in Figure 5.3,
which is the same as Figure 5.2 though for $A = 10$. As there is no exponential convergence, applying Eq. 5.3 and doing an exponential extrapolation on the $b$ coefficients calculated for $A = 10$ is not necessarily indicative of the coefficient as calculated by the interaction, and therefore no extrapolation was done and $A = 10$ was removed from any further analysis.

![IMME B Coefficients for $A = 10$](image)

Figure 5.3: IMME $b$ coefficient calculated for $A = 10$ as a function of $e_{\text{max}}$ ranging from $e_{\text{max}} = 6$ through $e_{\text{max}} = 12$ in order to check convergence.

### 5.2.3 IMME $c$ Coefficient Convergence

In addition to studying the $b$ coefficient, the $c$ coefficient was also calculated for each $e_{\text{max}}$. Figure 5.4 shows the $c$ coefficient plotted against $e_{\text{max}}$ for $A = 34$. The remaining $c$ coefficients can be found in Appendix J.

Taking a closer look at Figure 5.4 as well as the $c$ coefficients for other masses shown in Appendix J, it can be seen that while some masses appear to have $c$ coefficient converging with $e_{\text{max}}$, there are many which do not. As there was no consistent convergence between masses to implement convergence, no extrapolation to $e_{\text{max}} \to \infty$ was done. For further analysis, $e_{\text{max}} = 12$ was used and that the calculation may not be fully converged was taken
Figure 5.4: IMME $c$ coefficient calculated for $A = 34$ as a function of $e_{max}$ ranging from $e_{max} = 6$ through $e_{max} = 12$ in order to check convergence.

However, as with the $b$ coefficient there were some masses which did not give any sense of convergence, or even constancy in the values with increasing $e_{max}$. In order to make justified claims that the calculations being used were at least somewhat indicative of the interactions used, $A = 10$ and $A = 74$ needed to be removed from the sample. The plots of these $c$ coefficients are shown in Figure 5.5, and it can be seen very clearly that there is no sense of convergence with increasing $e_{max}$. The resulting masses used for analysis are in the range $A = \{14 : 70\}$.

5.3 Trends in the IMME Coefficients

As can be seen in the plots of convergence above there is significant deviation, even in the converged calculations, from experiment. As the calculations being done are \textit{ab initio}, this is expected, though it means that an individual $b$ or $c$ coefficient may not give much indication of how well \textit{ab initio} methods calculate ISB in the nuclear potential as well as studying
general patterns systematically. Specifically, by studying trends in the coefficients rather than looking at them individually, systematic effects in the interactions can be identified and studied.

### 5.3.1 Trends in the IMME $b$ Coefficient

In order to study systematic effects, the extrapolated values for the $b$ coefficients, as discussed earlier, were taken and plotted as a function of mass. This is seen in Figure 5.6, where the extrapolated values are plotted alongside experiment as well as two Coulomb estimates. The two charged sphere estimates are from a uniformly charged sphere (Appendix G), and a spherical nucleus with a WS charge density (Appendix H). These estimates were done as the IMME is motivated by a first order Coulomb expansion, and the most clear source of ISB in the nuclear potential is the electromagnetic repulsion between protons.

Figure 5.6 shows that the calculated $b$ coefficients over the entire mass range ($A = \{14 : 74\}$) systematically follow both the experimentally measured values and the WS estimate. Matching the WS estimate is an important first step in ensuring that the ab initio calculations are not significantly erroneous due to the nature of the IMME, and without this a reevaluation...
Figure 5.6: IMME $b$ coefficients as a function of mass plotted with $b$ coefficient calculated with only contributions from charged spheres.

of the calculation method would be necessary. That the $b$ coefficients agree so well with the WS estimate gives confidence to the assertion that the $b$ coefficient is dominated by the two-body Coulomb forces between protons [20].

Looking closer at Figure 5.6 shows that there does seem to be some deviation from experiment and the Coulomb estimates around $A = 14$ as well as $A = 40$. These two masses occur near HO shell closures, with $A = 14$ including nuclei with $N$ or $Z = 8$, the closure of the $p$ shell, and $A = 38, 42$ including nuclei with $N$ or $Z = 20$, the closure of the $sd$-shell. From this, it looks like there are effects caused by the HO shell closures which need to be investigated.

5.3.2 Trends in the IMME $c$ Coefficient

As there was no systematic convergence and therefore no extrapolation to $e_{max} \to \infty$ with the $c$ coefficient, $e_{max} = 12$ values were plotted as a function of mass. With no extrapolation, analysis of the $c$ coefficient must be done with the understanding that the values are estimates.
of the interactions and not their converged values. However, there was reasonable confidence in the $c$ coefficients at $e_{\text{max}} = 12$ as the mass excesses had converged, and the $c$ coefficients kept for analysis were not changing significantly with $e_{\text{max}}$. Plotting these values as a function of mass gives Figure 5.7.

![IMME c Coefficients](image)

Figure 5.7: IMME $c$ coefficients as a function of mass plotted with $c$ coefficient calculated with only contributions from charged spheres.

The trends seen in the $b$ coefficient (Figure 5.6) is also reproduced for the $c$ coefficient in Figure 5.7 though to a much greater degree. The calculated $c$ coefficients align with both experiment and the charged sphere estimates well, but disagree with values too large at HO shell closures. This reinforces that the effects of shell closures need to be investigated further.

### 5.4 Valence Space Decoupling

As it is seen that deviations occur at the closures of HO shells, these need to be investigated. In the VS-IMSRG many-body method there is a decoupling of the valence space which can be adjusted. As the valence space is different for each nucleus, the valence space being decoupled was set for each nucleus individually in order to provide the most accurate
calculation of the binding energy possible. However, because this causes nucleon shells to be decoupled separately, for nuclei at the HO shell closures, the protons and neutrons would be decoupled differently. This is because for nuclei like $^{38}\text{Ca}$, which has a completely full $sd$-shell of protons (20) and an open $sd$-shell of neutrons (18), the decoupling scheme where nucleon shells are decoupled separately would result in a decoupled $sd$-shell of neutrons and no decoupled valence space for protons. Denoted $0\hbar\omega$-shell decoupling, this decoupling scheme is shown pictorially for $^{38}\text{Ca}$ in Figure 5.8(a).

![Figure 5.8: Nucleons of $^{38}\text{Ca}$ shown with different choices of valence space decoupling.](image)

The other decoupling scheme, denoted by the shell being decoupled, is where the valence space is forced to be the same between the proton and neutron shells. Shown in Figure 5.8(b), this would cause the completely full $sd$-shell of protons in $^{38}\text{Ca}$ to be decoupled and treated as a valence space, albeit still with only one configuration of protons. In this configuration, the valence space decoupled can be written explicitly as the $p$-shell for $A = \{10,14\}$, the $sd$-shell for $A = \{18,22,26,30,34,38\}$, and the $fp$-shell for $A \geq 42$. While this may not result in the most accurate calculation for each nucleus, it does result in consistency for the entire IAT and therefore should mitigate some of the effects seen in Figure 5.6 and Figure 5.7 due to the HO shell closures.
5.5 Convergence of Calculations with Consistent Decoupling

As with the $0\hbar\omega$-shell decoupling, it is crucial that the calculations converge using the other decoupling scheme. In order to ensure this, the same process was used where binding energies, converted to mass excesses, were calculated for each member of the IAT, for all masses, at $e_{\text{max}} = \{6, 8, 10, 12\}$ and tested for convergence. These were then used to calculate IMME $b$ and $c$ coefficients, which were tested for convergence as well using the same methods as above.

5.5.1 Mass Excess Convergence with Consistent Decoupling

After calculating binding energies using the consistent decoupling scheme, mass excesses were calculated using Eqs. 5.1 and 5.2. The convergence of mass excesses calculated using the consistent decoupling scheme for $A = 38$ and $A = 42$ are shown in Figure 5.9 and Figure 5.10 respectively. These were chosen because they show the effects caused by the consistent decoupling scheme on the mass excesses as well as the relative significance of the effects between nearly full and nearly empty HO shells.

The consistent decoupling between shells reduces the mass excess, or increases the binding, in all cases, though the significance of the effects are seen to be greater near full shells rather than shells with few nucleons. In $A = 38$, the effects of the decoupling scheme can be seen visibly while in $A = 42$ the effects are much more subtle. The same can be seen in Appendix F for $A = 14$ and $A = 18$, which surround the closure of the $p$-shell.

One sanity check done was to ensure that the calculated values for mass excess for the $T_z = 0$ nucleus did not change with the different decoupling scheme as the new scheme did not change the decoupling for these nuclei. In $T_z = 0$ nuclei, $N = Z$ and both nucleons have the same valence space decoupled in both decoupling schemes.

5.5.2 IMME $b$ Coefficient Convergence with Consistent Decoupling

Again using the same method for looking at the convergence of the $b$ coefficients, the convergences for $A = 38$ and $A = 42$ can be seen in Figure 5.11.
Figure 5.9: Mass excesses of the $A = 38$ IAT calculated using both EM1.8/2.0 and N2LOsat plotted with experimental values. Solid coloured lines represent an exponential extrapolation of the $e_{\text{max}} = \{8, 10, 12\}$ points.

Figure 5.10: Mass excesses of the $A = 42$ IAT calculated using both EM1.8/2.0 and N2LOsat plotted with experimental values. Solid coloured lines represent an exponential extrapolation of the $e_{\text{max}} = \{8, 10, 12\}$ points.
Figure 5.11: IMME $b$ coefficient calculated for $A = 38, 42$ as a function of $e_{\text{max}}$ ranging from $e_{\text{max}} = 6$ through $e_{\text{max}} = 12$ in order to check convergence. Solid coloured lines represent an exponential extrapolation of the $e_{\text{max}} = \{8, 10, 12\}$ points.

Figure 5.11 shows that the effects of the decoupling scheme reduces the $b$ coefficient for all cases at shell closures, and reduces it significantly for the cases where the valence space is nearly full. This can also be seen in the closure of the $p$-shell in Appendix I. Despite this, there is clearly no change in the shape of the convergence with the decoupling scheme.

The improvement in both the rate of convergence and the proximity to the experimental value indicate that the consistent decoupling method is a more accurate way to look at systematic effects of ISB, but the $b$ coefficient is not enough to confidently state that the decoupling scheme is a significant factor.

5.5.3 IMME $c$ Coefficient Convergence with Consistent Decoupling

Using the new decoupling scheme, the $c$ coefficients were also calculated as above. These are shown in Figure 5.12, again as these two masses surround the closure of the $sd$-shell.

Figure 5.12 shows similar effects with the $c$ coefficients as Figure 5.11 showed with the $b$; the effect of the consistent decoupling scheme is to lower the $c$ coefficients, slightly improve the trend of convergence, and to make the $c$ coefficient significantly closer to the experimental value. Additionally, it is seen that for the masses where the shells are almost full the effect
Figure 5.12: IMME \( c \) coefficient calculated for \( A = 38, 42 \) as a function of \( e_{\text{max}} \) ranging from \( e_{\text{max}} = 6 \) through \( e_{\text{max}} = 12 \) in order to check convergence.

is significantly greater than the effects on masses at the beginning of shells.

As the effects of the decoupling scheme are the same for the \( c \) coefficient as they are for the \( b \) coefficient, the implications are the same as well. It seems that by looking at the coefficients individually that the consistent decoupling scheme significantly improves the deviations seen in Figure 5.6 and Figure 5.7 around shell closures.

5.6 Trends in the IMME Coefficients with Consistent Decoupling

Though both the \( b \) and \( c \) coefficient convergence plots indicate that the consistent decoupling scheme provides a more accurate representation of both the interaction and the IMME coefficients, this claim cannot be fully made until the consistent decoupling is applied systematically and studied. As such, the same trend analysis was done for the consistent decoupling scheme as was done for the 0\( \hbar \omega \)-shell scheme for both the \( b \) and \( c \) coefficients. These were also compared to the 0\( \hbar \omega \)-shell decoupling scheme directly to give insight into how significant the decoupling scheme is.
5.6.1 Trends in the IMME \( b \) Coefficient with Consistent Decoupling

In studying the \( b \) coefficients, the same extrapolation (Eq. 5.4) was used for the consistent decoupling scheme in order to provide the \( b \) coefficient as \( e_{\text{max}} \to \infty \). This allows the four consistent decoupling \( b \) coefficients to be added to Figure 5.6, resulting in Figure 5.13.

![IMME \( b \) Coefficients](image)

Figure 5.13: IMME \( b \) coefficients calculated using both decoupling schemes plotted as a function of mass with \( b \) coefficient calculated with only contributions from charged spheres.

In Figure 5.13 there is no significant difference in the \( b \) coefficients with the consistent decoupling scheme, though there is slight improvement in all four cases. Because the difference in the decoupling scheme does not change the trend, both decoupling schemes will be kept for further analysis.

Because of the scale of the \( b \) coefficients, it appears in Figure 5.13 that the calculated values for the \( b \) coefficients align extremely well with the experimental values, and by subtracting off the WS sphere estimate more structure in the trend can be seen. Figure 5.14 shows the \( b \) coefficients for both \textit{ab initio} methods as well as experiment with the WS sphere estimate subtracted off.
Figure 5.14: IMME $b$ coefficients as a function of mass with contribution from a charged sphere with a Woods Saxon charge density subtracted off.

With Figure 5.14 more discernible structure can be seen. Overall, remarkable agreement between experimental and theoretical coefficients can be seen indicating that systematic effects from the $ab\ initio$ methods have effectively been subtracted off.

More prominent though is that there does appear to be some additional structure to the shape of the curve overall; there is an overall negative slope on each of the five sets of values plotted with increasing mass. Before the closure of the $sd$-shell, the $b$ coefficients are predominantly positive, or slightly negative, but around the closure of the $sd$-shell there is a significant drop in the $b$ coefficients calculated using $ab\ initio$ methods, but not a steep drop in the experimental values. The overall shape of the curve implies that there are other $A$-dependent, non-shell dependent ISB forces. However, the steep drop in the $ab\ initio$ calculated values implies that there is a significant difference in the way ISB effects are treated between the $sd$-shell and the $fp$-shell. Despite this, removing the $A = 38$ point reduces the steepness of the drop, and as the VS-IMSRG method is known to struggle near HO shell closures [50], there cannot be any strong conclusions drawn from this.
While this is notable, there appear to be significant peaks in the differences between the calculated values from \textit{ab initio} methods and experiment around shell closures. This can be seen clearer by looking at the residuals of the \textit{ab initio} calculations in Figure 5.15.

![IMME b Coefficients Residuals](image)

**Figure 5.15:** IMME $b$ coefficient residuals as a function of mass.

The effects of shell closures are even more prominent in Figure 5.15 and there are significant changes between nuclei calculated in the middle of shells and those calculated near shell closures. While the $b$ coefficients for mid-shell nuclei are reproduced well compared to experiment, there are significant peaks around shell closures and again at $A = 64$. These deviations from experiment are expected as the VS-IMSRG many body method is known to provide more accurate calculations in the middle of shells and struggles near closures [50].

Though initially unexpected due to there being no shell closure at $A = 64$ around the $N = Z$ line, a closer analysis of the nuclear shell model explains what appears to be a similar effect at this mass. Due to the $\ell \cdot s$ splitting, the $g_{9/2}$ shell (refer to Figure 2.3) has a reduced energy and appears to lie firmly in the $fp$-shell. Due to this effect, the VS-IMSRG method has been shown to become less accurate at $N, Z \gtrsim 30 - 35$ [50].
Though explanations, at least with some level of confidence, can be made for the trends seen in the $b$ coefficients above, there is one significant trend which is not immediately obvious and is extremely surprising. Based on the charge radii reproduced by the EM1.8/2.0 interaction as reported in [104], and the known dependence of the IMME $b$ coefficient on the charge radius (e.g. [78]), the EM1.8/2.0 interaction fits experimental data too well. With the IMME $b$ coefficient changing proportional to $1/R$ as $A$ increases, it is estimated that the $b$ coefficient produced by the EM1.8/2.0 interaction should be off by $\sim 10\%$, an effect which is not seen. One possible explanation for this is that the Coulomb shift in the wavefunctions caused by the small radii produced by the EM1.8/2.0 interaction offsets the effects of the radius when looking at the $b$ coefficient. Further work is necessary for testing this.

5.6.2 Trends in the IMME $c$ Coefficient with Consistent Decoupling

Though there were a few cases where the consistent decoupling scheme improved convergence, there was still no systematic convergence, and so the $e_{\max} = 12$ value for the calculations were used to study the consistent decoupling scheme as well. Adding these calculated to Figure 5.7 results in Figure 5.16.

The result of adding the consistent decoupling scheme is significant, with both of the major peaks being reduced and almost entirely eliminated. It is Figure 5.16 which gives the most confidence that the consistent decoupling scheme is needed to go forward and look at ISB effects in nuclear interactions. Removing the $0\hbar\omega$-shell decoupling from Figure 5.16 decreases the plot range and zooms in on the structure of the coefficients significantly, resulting in Figure 5.17.

By zooming in on the $c$ coefficients as a function of mass, it can be seen that while the general trend of the calculated values does agree with the charged sphere estimates, the WS charge density only account for between one third and one half of the $c$ coefficient. While the IMME is motivated by the first order Coulomb expansion and it would be naively expected that the WS charge density would account for more than this, it can be noted that the experimentally measured $c$ coefficients are also systematically higher than the WS estimate.
Figure 5.16: IMME $c$ coefficients calculated using both decoupling schemes plotted as a function of mass with $c$ coefficient calculated with only contributions from charged spheres.

Figure 5.17: IMME $c$ coefficients calculated using the consistent decoupling scheme plotted as a function of mass with $c$ coefficient calculated with only contributions from charged spheres.
This gives validation to the assertion that the $c$ coefficient can be attributed to the difference in the $pp$ and $nn$ forces [20], as the Coulomb interaction does not account for the entirety of the $c$ coefficient.

Additionally, there can be seen some additional effects near shell closures. This can be seen more clearly by removing the WS contribution from the *ab initio* and experimental values, which results in Figure 5.18

![Shifted IMME $c$ Coefficients](image)

Figure 5.18: IMME $c$ coefficients as a function of mass with contribution from a charged sphere with a Woods Saxon charge density subtracted off.

Looking at Figure 5.18 it becomes more clear that the experimentally measured values are systematically larger than the WS estimate. Additionally, the $c$ coefficients calculated using *ab initio* methods are significantly larger than the experimental values. For the EM1.8/2.0 interaction, deviation from the WS estimate for the calculated values are between $\sim 2$ and $\sim 4$ times larger than the same for the experimental values. As the $c$ coefficient has been attributed to the difference in the $pp$ and $nn$ forces [20], one logical conclusion is that the *ab initio* calculations overestimate that effect, though no firm statement can be made to this effect.
Unlike with the $b$ coefficient, there are no significant effects in the $c$ coefficient around $A = 64$ in the $ab\ initio$ calculations, though these effects are seen experimentally.
CHAPTER 6
SUMMARY AND CONCLUSIONS

Testing the unitarity of the CKM matrix through superallowed $0^+ \rightarrow 0^+ \beta$ decay systems is an active area of research in nuclear physics. This is because measurements of superallowed $\beta$ decay provide the most precise determination of the up-down element of the CKM quark mixing matrix, $V_{ud}$. However, the error budget on the calculation of $V_{ud}$ is dominated by theoretical corrections, and one correction in particular, the isospin symmetry breaking (ISB) correction ($\delta_C$), is determined through complex theoretical nuclear structure calculations.

Nuclear many body methods, specifically the valence-space in-medium similarity renormalization group (VS-IMSRG) method, paired with interactions from chiral effective field theory provide an ab initio approach for the calculation of ISB corrections. While these ab initio methods include ISB terms in the interactions, they need to be benchmarked against something known to be sensitive to subtle changes in ISB terms before they can be used for tests of the SM. These tests would allow ISB to be tested in ab initio methods, but also for problems or areas of improvement, to be identified with the intent to begin quantifying uncertainty.

In this work, the isobaric multiplet mass equation (IMME), a quadratic equation motivated from a first order perturbative expansion of the Coulomb potential, was used to benchmark ab initio methods against both experimental values and charged sphere estimates. Isobaric analogue triplets of interest to be studied include masses $A = 10$ through $A = 74$, every four, because these isobaric analogue states are connected via superallowed $\beta$ decay, thereby allowing the Fermi coupling constant of the weak interaction to be isolated.

The IMME coefficients for these isobaric analogue triplets of interest were calculated using two different decoupling schemes, and while there should be no dependence on the decoupling, significant dependence was found. The first decoupling scheme, which decouples the valence
space for each nucleon shell independently and provides the most accurate representation of an individual nucleus, was found to be inconsistent for the IMME coefficient, and resulted in significant deviation from experiment. By forcing the valence space to be the same for both protons and neutrons, consistency was achieved and the \textit{ab initio} values systematically followed trends seen in both experiment and charged sphere estimates.

Further analysis on the coefficients showned that calculations of the $b$ coefficient were significantly better for nuclei far from closed shells and were systematically high near shell closures. This result was expected at the outset because the VS-IMSRG method has been known to work better in the centre of shells compared to near closures. \textit{Ab initio} calculations of the $c$ coefficient followed the trends of experiment and the charged sphere estimates very well though with a systematic shift. With the $c$ coefficient, both \textit{ab initio} methods as well as experiment produced systematically higher values than the charged sphere estimates indicating non-negligible ISB terms separate from the first order Coulomb potential. While a reasonable explanation would be an overestimate of the difference between the $pp$ and $nn$ two-body forces, no firm assertion can be made at this time to that effect.

One significant unexpected result which arose was how well the EM1.8/2.0 interaction calculated the IMME coefficients. Due to the motivation of the IMME coming from a first order expansion of the Coulomb interaction and the systematically small charge radii of the interaction, the expectation was that the magnitude of the IMME coefficients would be overpredicted by $\sim 10\%$, but this effect was not seen in the $b$ coefficient. However, this was seen in the $c$ coefficient, at least when compared only to the N2LOsat interaction. Further work, such as calculating the expectation value of the Coulomb operator using the \textit{ab initio} method, is necessary to determine why this effect was not seen. This is however, outside the scope of this current work.

Overall, from the results of the systematic study of the IMME coefficients shown in this Thesis, there is reason to doubt that calculations of $\delta C$ using \textit{ab initio} methods would be accurate. Along with the lack of convergence in the $c$ coefficient with increasing $e_{\text{max}}$, this is
because there was significant dependence on the decoupling scheme used in the VS-IMSRG method on the calculation of the $c$ coefficient, while there ideally should be no dependence. Additionally, the EM1.8/2.0 interaction systematically reproduced the $b$ coefficient well despite producing charge radii which are too small. While more work needs to be done in order to begin quantifying the uncertainty in \textit{ab initio} methods, these two factors reduce the confidence in these calculations further. The results of this work show that significant improvements in theoretical methods still need to be made in order for \textit{ab initio} methods to be used confidently for tests of the Standard Model.
APPENDIX A
DERIVATION OF THE $\beta$ DECAY CONSTANT

This derivation is an adaptation taken from [12, 117]. Starting with Fermi’s Golden Rule

$$\lambda = \frac{2\pi}{\hbar} |M_{fi}|^2 \frac{dn}{dE}, \quad (A.1)$$

the density of states $\frac{dn}{dE}$ can be expanded by considering that it must include all possible states of the electron (positron) and anti-neutrino (neutrino). Normalizing these particles in a box with arbitrary volume $V$ the number of states can be written as

$$n = \frac{V^2}{(2\pi \hbar)^6} \int p_e^2 dp_e \int p_n^2 dp_n \int d\Omega_e \int d\Omega_\nu, \quad (A.2)$$

where both of the $\Omega$ integrals simplify to $4\pi$ if all emitted particles are allowed to be emitted in all directions. This allows the differential form of Eq. A.2 to be rewritten as

$$dn = \frac{(4\pi V)^2}{(2\pi \hbar)^6} p_e^2 p_\nu d\Omega_e d\Omega_\nu. \quad (A.3)$$

Remembering that in Fermi’s theory the neutrino is massless, the momentum and energy are related as

$$p_\nu = \frac{1}{c} E_\nu, \quad (A.4)$$

and the density of states can be written as

$$\frac{dn}{dE} = \frac{(4\pi V)^2}{(2\pi \hbar)^6 c^3} p_e^2 (E - E_e)^2 dE_e. \quad (A.5)$$

This makes the $\beta$ decay constant from Fermi’s Golden Rule

$$d\lambda = \frac{V^2}{2\pi^3 \hbar^7 c^3} |M_{fi}|^2 p_e^2 (E - E_e)^2 dE_e, \quad (A.6)$$

which still relies on an arbitrary volume $V$. This volume disappears when considering that the transition matrix depends on the nuclear wave functions. Assuming that the two particles are emitted in all directions isotropically as was done for the $\Omega$ integrals, the wave functions
can be written as in Eqs. A.7 and A.8 for the neutrino and electron respectively.

\[
\psi_\nu(\vec{r}_\nu) = \frac{1}{\sqrt{V}} e^{i\vec{p}_\nu \cdot \vec{r}_\nu} \quad (A.7)
\]

\[
\psi_e(\vec{r}_e) = \frac{1}{\sqrt{V}} e^{i\vec{p}_e \cdot \vec{r}_e} (F(Z_D, p_e))^{1/2} \quad (A.8)
\]

The two wave functions look identical aside from the change in coordinates representing the two individual particles and the Fermi function on the electron wave function which accounts for the Coulomb effects of the charged particle. The Fermi function, when treated relativistically, has the form as in Eq. A.9

\[
F(Z_D, p_e) = 2(1 + \gamma) \left(\frac{2p_e R}{\hbar}\right)^{2\gamma-2} e^{\pi\eta} \frac{\left|\Gamma(\gamma + i\eta)\right|^2}{\left|\Gamma(2\gamma + 1)\right|^2},
\]

where \(\gamma = \sqrt{1 - (\alpha Z_D)^2}\), \(\eta = \mp \frac{Z_D e^2}{p_e c}\) for \(\beta^\pm\) decay, and \(\Gamma\) is the complex gamma function. Including the Fermi function into the wave function for the electron allows the coupling to be removed from the transition matrix \(|M_{fi}|^2 = g^2 \left|\overline{M}_{fi}\right|^2\) where \(\left|\overline{M}_{fi}\right|\) does not depend on the electron energy or momentum. This allows the decay constant to finally be written as

\[
\lambda = \frac{g^2 \left|\overline{M}_{fi}\right|^2}{2\pi^3 \hbar^7 c^3} \int F(Z_D, p_e) p_e^2 (E - E_e)^2 dp_e. \quad (A.10)
\]

The integral in Eq. A.10, along with constants to make it dimensionless as in Eq. A.11, is a dimensionless phase integral. Including this allows the decay constant to be written as in Eq. A.12, which is how it is used in the Fermi theory.

\[
f = f(Z_D, E) = \frac{1}{(m_e c)^3 (m_e c^2)^2} \int F(Z_D, p_e) p_e^2 (E - E_e)^2 dp_e \quad (A.11)
\]

\[
\lambda = \frac{g^2 \left|\overline{M}_{fi}\right|^2 m_e^5 c^4}{2\pi^3 \hbar^7} f(Z_D, E) \quad (A.12)
\]
APPENDIX B
DERIVATION OF THE IMME

This derivation was adapted from [78] with some interpretation from [118]. The Coulomb potential is a two-body interaction between two charged particles, and in atomic units ($\hbar = m_e = e = k = 1$, where $k$ is the Coulomb constant), can be written as

$$V = \sum_{i<j} \frac{Q_i Q_j}{|\vec{r}_i - \vec{r}_j|},$$

(B.1)

where $Q$ represents the charge of the particle in question and is a constant and $\vec{r}_i$ is a position vector. In the isospin formalism, the charge $Q$ can be written in terms of isospin projection as

$$Q_i = \frac{1}{2} - t_z(i),$$

(B.2)
as a proton with isospin projection of $-\frac{1}{2}$ will give a charge of 1 and a neutron with isospin projection of $+\frac{1}{2}$ will give a charge of zero. Using this formalism, the Coulomb potential can be written as

$$V = \sum_{i<j} \left( \frac{1}{2} - t_z(i) \right) \left( \frac{1}{2} - t_z(j) \right) \frac{1}{|\vec{r}_i - \vec{r}_j|},$$

(B.3)

By expanding the two charge terms, the potential can be written as

$$V = \sum_{i<j} \left( \frac{1}{4} - \frac{1}{2} (t_z(i) + t_z(j)) + t_z(i)t_z(j) \right) \frac{1}{|\vec{r}_i - \vec{r}_j|},$$

(B.4)

which naturally leads to the separation of terms

$$V = \sum_{q=0,1,2} V^{(q)},$$

(B.5)

where

$$V^{(0)} = \sum_{i<j} \left( \frac{1}{4} + \frac{1}{3} \vec{t}(i) \cdot \vec{t}(j) \right) \frac{1}{|\vec{r}_i - \vec{r}_j|},$$

(B.6)

$$V^{(1)} = \sum_{i<j} \frac{1}{2} (t_z(i) + t_z(j)) \frac{1}{|\vec{r}_i - \vec{r}_j|},$$

(B.7)
\[ V^{(2)} = \sum_{i<j} \left( t_z(i)t_z(j) - \frac{1}{3} \vec{t}(i) \cdot \vec{t}(j) \right) \frac{1}{|\vec{r}_i - \vec{r}_j|}. \]  

Eqs. B.6, B.7, and B.8 correspond to isoscalar, isovector, and isotensor terms with no \( T_z \) dependence, linear \( T_z \) dependence, and quadratic \( T_z \) dependence respectively. The \( \vec{t}(i) \cdot \vec{t}(j) \) terms in Eqs. B.6 and B.8 are included to satisfy the isoscalar and isotensor definitions and allow for the terms to be sorted by tensor rank and symmetry groups [119].

Using this form of the Coulomb potential, lowest order perturbation theory gives the shift in energy of an isobaric multiplet due to the electromagnetic potential as

\[ E(\alpha, T, T_z) = \langle \alpha, T, T_z \mid \sum_{q=0,1,2} V^{(q)} \mid \alpha, T, T_z \rangle. \]  

where \( \alpha \) is a placeholder representing quantum numbers in the state \((j, m, s, \text{etc.})\). The \( T_z \) dependence of the inner product can be removed using the Wigner-Eckart theorem [120, 121], allowing the expectation value to be written as a function of a 3-j symbol.

\[ E(\alpha, T, T_z) = \sum_{q=0,1,2} (-1)^{T_q-T_z} \left( \begin{array}{ccc} T & q & T \\ -T_z & 0 & T_z \end{array} \right) \langle \alpha, T \mid V^{(q)} \mid \alpha, T \rangle \]  

By writing it in this way, the 3-j symbol can be interpreted in terms of Clebsch-Gordon coefficients as

\[ \left( \begin{array}{ccc} T & q & T \\ -T_z & 0 & T_z \end{array} \right) = \frac{(-1)^{T-q-T_z}}{\sqrt{2T+1}} \langle T, T_z, q, 0 \mid T, T_z \rangle \]  

where the inner product at the end is the Clebsch-Gordon coefficient [122]. Using this form of the energy shift, the sum can be written explicitly, with the Clebsch-Gordon coefficients included, as

\[ E(\alpha, T, T_z) = E^{(0)}(\alpha, T) + E^{(1)}(\alpha, T)T_z + E^{(2)}(\alpha, T)(3T_z^2 - T(T + 1)) \]  

with

\[ E^{(0)} = \frac{1}{\sqrt{2T+1}} \langle \alpha, T \mid V^{(0)} \mid \alpha, T \rangle \]  

\[ E^{(1)} = \frac{1}{\sqrt{T(2T+1)(T+1)}} \langle \alpha, T \mid V^{(1)} \mid \alpha, T \rangle \]
\[ E^{(2)} = \frac{1}{\sqrt{T(2T+3)(2T+1)(T+1)(2T-1)}} \langle \alpha, T \parallel V^{(2)} \parallel \alpha, T \rangle. \]  

(B.15)

From here, the mass excess itself can be derived by adding the Coulomb shift to the calculation for charge independent mass excess as

\[ M(\alpha, T, T_z) = \frac{1}{2}(M_n + M_H)A + (M_n - M_H)T_z + \langle \alpha, T, T_z \parallel H_0 \parallel \alpha, T, T_z \rangle + E(\alpha, T, T_z) \quad (B.16) \]

where \( M_n \) and \( M_H \) are the mass excesses of the neutron and hydrogen respectively (i.e. \( M_n = m_n - 1 \) where \( m_n \) is the mass of a neutron in atomic mass units). The first two terms in Eq. B.16 account for the mass excesses of the constituent particles of the nucleus, the third accounts for the binding of a charge and isospin-independent nucleus, and the final term is the Coulomb correction derived above. This allows Eq. B.16 to be written more conveniently as

\[ M(\alpha, T, T_z) = a(\alpha, T) + b(\alpha, T)T_z + c(\alpha, T)T_z^2 \quad (B.17) \]

with coefficients

\[ a(\alpha, T) = \frac{1}{2}(M_n + M_H)A + \langle \alpha, T, T_z \parallel H_0 \parallel \alpha, T, T_z \rangle + E^{(0)}(\alpha, T) - T(T+1)E^{(2)}(\alpha, T) \quad (B.18) \]

\[ b(\alpha, T) = (M_n - M_H) - E^{(1)}(\alpha, T) \quad (B.19) \]

\[ c(\alpha, T) = 3E^{(2)}(\alpha, T). \quad (B.20) \]

where Eq. B.17 is the form known as the IMME.
APPENDIX C
EXAMPLE OF SRG FLOW

The most general case of a $2 \times 2$ matrix representation of a Hamiltonian guaranteed to have real eigenvalues is

$$H(s) = \begin{bmatrix} \epsilon_1(s) & V^*(s) \\ V(s) & \epsilon_2(s) \end{bmatrix}.$$  \hfill (C.1)

This can easily be split into its diagonal and off-diagonal parts ($H_d(s)$ and $H_{od}(s)$), which quickly shows that when the SRG is used to diagonalize the Hamiltonian, both of the limits in Eq. C.2 should be satisfied.

$$\lim_{s \to \infty} V(s) \to 0$$
$$\lim_{s \to \infty} V^*(s) \to 0$$ \hfill (C.2)

In order to do so, a generator needs to be specified. As the White generator is being used for the purposes of this Thesis, the White generator will be used for this example. The White generator needs to be anti-Hermitian, and can be written explicitly for this Hamiltonian as

$$\eta(s) := \frac{1}{\epsilon_2 - \epsilon_1} \begin{bmatrix} 0 & -V^*(s) \\ V(s) & 0 \end{bmatrix}.$$  \hfill (C.3)

$$\eta^\dagger(s) = \frac{1}{\epsilon_2 - \epsilon_1} \begin{bmatrix} 0 & V^*(s) \\ -V(s) & 0 \end{bmatrix} = -\eta(s).$$ \hfill (C.4)

Using these two definitions and the SRG flow equation

$$\frac{d}{ds} H(s) = [\eta(s), H(s)],$$ \hfill (C.5)
a set of coupled differential equations can be found with respect to the flow parameter $s$. In order to find these differential equations, Eq. C.5 must be solved, and is done so in Eq. C.6.

\[
\begin{bmatrix}
\dot{\epsilon}_1(s) & \dot{V}^*(s) \\
\dot{V}(s) & \dot{\epsilon}_2(s)
\end{bmatrix} = \frac{1}{\epsilon_2(s) - \epsilon_1(s)} \left( \begin{bmatrix}
0 & -V^*(s) \\
V(s) & 0
\end{bmatrix} \begin{bmatrix}
\epsilon_1(s) & V^*(s) \\
V(s) & \epsilon_2(s)
\end{bmatrix} - \begin{bmatrix}
\epsilon_1(s) & V^*(s) \\
V(s) & \epsilon_2(s)
\end{bmatrix} \begin{bmatrix}
0 & -V^*(s) \\
V(s) & 0
\end{bmatrix} \right)
\]

\[
= \frac{1}{\epsilon_2(s) - \epsilon_1(s)} \begin{bmatrix}
-2V^2 & -V^*(s) (\epsilon_2(s) - \epsilon_1(s)) \\
V(s)(\epsilon_1(s) - \epsilon_2(s)) & 2V^2
\end{bmatrix}
\]

(C.6)

The final line of Eq. C.6 gives four, first order, coupled differential equations which when solved give the evolution of the Hamiltonian as a function of the flow parameter $s$. Simply reading off each component of the matrices gives these four differential equations, written explicitly in Eq. C.7.

\[
\dot{\epsilon}_1(s) = -\frac{2|V(s)|^2}{\epsilon_2(s) - \epsilon_1(s)}
\]

\[
\dot{\epsilon}_2(s) = -\frac{2|V(s)|^2}{\epsilon_2(s) - \epsilon_1(s)}
\]

\[
\dot{V}^*(s) = -V^*(s)
\]

\[
\dot{V}(s) = -V(s)
\]

(C.7)

The bottom two of these differential equations are well behaved as they send the off-diagonal part of the Hamiltonian to zero with increasing $s$, which mean as $s \to \infty, H_{od}(s) \to 0$. These two equations are decoupled from the first two and can be solved explicitly as in Eq. C.8.

\[
V(s) = V(0)e^{-s}
\]

\[
V^*(s) = V^*(0)e^{-s}
\]

(C.8)
Eq. C.8 allows for the other two differential equations to be simplified, and written as in Eq. C.9.

\[
\begin{align*}
\dot{\epsilon}_1(s) &= \frac{-2e^{-2s}|V(0)|^2}{\epsilon_2(s) - \epsilon_1(s)} \\
\dot{\epsilon}_2(s) &= \frac{2e^{-2s}|V(0)|^2}{\epsilon_2(s) - \epsilon_1(s)}
\end{align*}
\]  

(C.9)

Now the issue comes with solving these two coupled first ordered differential equations. By making a simple change of variables given by Eq. C.10 these two differential equations become decoupled, with one becoming trivial as well.

\[
E(s) := \frac{1}{2} (\epsilon_1(s) + \epsilon_2(s)) \\
\Delta(s) := \epsilon_2(s) - \epsilon_1(s)
\]

(C.10)

Using this substitution, the two differential equations become

\[
\begin{align*}
\dot{E}(s) &= 0 \\
\dot{\Delta}(s) &= -\frac{4e^{-2s}|V(0)|^2}{\Delta(s)}
\end{align*}
\]

(C.11)

The first of these two differential equations is trivial, and simply states that the sum of \(\epsilon_1(s)\) and \(\epsilon_2(s)\) is a constant during the continuous transformation. The second differential equation is not so trivial, but can be solved explicitly for the function \(\Delta(s)\).

\[
\begin{align*}
\Delta(s)\dot{\Delta}(s) &= -4e^{-2s}|V(0)|^2 \\
\frac{d}{ds}(\Delta(s)^2) &= -8e^{-2s}|V(0)|^2 \\
\Delta(s)^2 &= -8|V(0)|^2 \int e^{-2s}ds \\
\Delta(s)^2 &= -4|V(0)|^2 e^{-2s} + C
\end{align*}
\]  

(C.12)
Using the definition of \( \Delta(s) \) given in Eq. C.10, the initial condition \( (s = 0) \) can be used to determine the constant \( C \). The calculation of the coefficient \( C \) is done in Eq. C.13.

\[
\Delta(0)^2 = [\epsilon_2(0) - \epsilon_1(0)]^2 \\
= -4 |V(0)|^2 + C \\
\implies C = [\epsilon_2(0) - \epsilon_1(s)]^2 + 4 |V(0)|^2 \quad (C.13)
\]

Applying the integration constant \( C \) from Eq. C.13 to Eq. C.12, an equation for \( \Delta(s) \) can be solved. Using this, as well as Eq. C.10, the three parameters can be written to flow with \( s \) as shown in Eq. C.14.

\[
\epsilon_1(s) = \bar{E}(s) - \frac{1}{2} \Delta(s) \\
= \frac{1}{2} [\epsilon_1(0) + \epsilon_2(0)] - \frac{1}{2} \sqrt{[\epsilon_2(0) - \epsilon_1(0)]^2 + 4 |V(0)|^2 (1 - e^{-2s})} \\
\epsilon_2(s) = \bar{E}(s) + \frac{1}{2} \Delta(s) \\
= \frac{1}{2} [\epsilon_1(0) + \epsilon_2(0)] + \frac{1}{2} \sqrt{[\epsilon_2(0) - \epsilon_1(0)]^2 + 4 |V(0)|^2 (1 - e^{-2s})} \quad (C.14)
\]

\[
V(s) = V(0)e^{-s} \\
V^*(s) = V^*(0)e^{-s}
\]

This means that rather than doing the diagonalization of the matrix itself, these four equations can be solved for \( s \to \infty \) and the resulting expressions used as a diagonal form of the original matrix. It is worth noting explicitly that the only \( s \) dependence in Eq. C.14 is in decaying exponentials, which will all go to zero as \( s \to \infty \). More importantly, these four equations are all fully decoupled from one another, and only rely on initial values.
APPENDIX D

WRAPPER FOR IMSRG AND NUSHELLX@MSU

# This code is set up such that a single command from the command line or a bash script will do everything and output the final binding energy of the lowest 0+ state in the nucleus specified.
# The input has the form
"python3 RunThis.py A Z e VS"

where A is the mass, Z is the proton number, e is emax, and VS is the valence space used in the VS–IMSRG code. Options for VS are 'Ohw–shell', 'p–shell', 'sd–shell', etc.

--Matthew S. Martin
Colorado School of Mines, 2018

# Imports packages relevant
import os
import time
import timeit
from sys import argv

# Starts a timer so you can see how long it took
start = timeit.default_timer()

# List of elements for reference

# Convert the command line arguments to variables
A = argv[1]
Z = argv[2]
e = argv[3]
VS = argv[4]
interaction = 'N2LOsat' # Uncomment for N2LOsat
```python
# interaction = 'EM1.8_2.0'  # Uncomment for EM1.8/2.0

# Calls the VS–IMSRG code and gives the command line arguments
os.system("python3 MattRun.py "+str(A)+" "+str(Z)+" "+str(e)+" "+str(VS))

# Converts Z and e to lists for looping over
# Allows running of multiple cases with one command line argument
Z = Z.split(' , ')
e = e.split(' , ')

# This is the loop which goes through and takes the output from the
# VS–IMSRG code and copies specific files, runs NuShellX@MSU, and
gives the final binding energy
for z in Z:
    z = int(z)
ele = ELEM[z]
    for E in e:
        # Makes a directory (if necessary) to do the shell model
diagonalization for the specific case
        os.system("mkdir -p ~/Documents/Theory/Shell_Model/Files"+str(A)+"/"+str(A)+str(ele)+str(E)+"_imsrg")

# Copies .int and .sp files created by the VS–IMSRG code to the
# new directory. Interaction chooses which line to run
if interaction == 'N2LOsat':
    os.system("cp output/"+str(VS)+"_N2LOsat_magnus_"+str(ele)+str(A)+"_E14_s500_hw20_A"+str(A)+".*/Documents/Theory/Shell_Model/Files"+str(A)+"/"+str(A)+str(ele)+str(E)+"_imsrg")  # N2LOsat
elif interaction == 'EM1.8_2.0':
    os.system("cp output/"+str(VS)+"_EM1.8_2.0_magnus_"+str(ele)+str(A)+"_E16_s500_hw16_A"+str(A)+".*/Documents/Theory/Shell_Model/Files"+str(A)+"/"+str(A)+str(ele)+str(E)+"_imsrg")  # EM1.8/2.0

# Changes directory to the folder for shell model diagonalization
os.chdir("~/Documents/Theory/Shell_Model/Files"+str(A)+"/"+str(A)+str(ele)+str(E)+"_imsrg")

# Renames the two files to imsrg.int and imsrg.sp
os.system("mv *.int imsrg.int")  # *int is the interaction file
os.system("mv *.sp imsrg.sp")  # *sp is the model space file

# Creates *ans file with options for shell model diagonalization
ansfile = "−\nlpe\nimsrg\nn\nimsrg\n"+str(z)+"\n"+str(A)+"\n0,4,1\n2\n−\nnst"
```

82
D.72  `textfile = open(str(A)+str(ele)+".ans", 'w')`
D.73  `textfile = textfile.write(ansfile)`
D.74
D.75  `# Runs the shell model calculation with the .ans file`  
D.76  `os.system("shell "+str(A)+str(ele)+".ans")`
D.77  `# Speeds up calculation by suppressing high energy states`  
D.78  `os.system("sed -i -i 's/10/1/g' *.neig")`
D.79  `# Runs the .bat file and produces the energy`  
D.80  `os.system("bash "+str(A)+str(ele)+".bat")`
D.81
D.82
D.83  `# At this point the binding energy has been calculated and now it`  
D.84  `# is just getting the energy out and storing it to file along with`  
D.85  `# other appropriate information`  
D.86
D.87
D.88  `# Grabs the bound state energy from the .int file and stores it`  
D.89  `intfile = open("imsrg.int", 'r')`
D.90  `intfile = intfile.readlines()`  
D.91  `boundstate = float(intfile[4][18:].replace(" ",""))`
D.92  `print(boundstate)  # Sanity check to make sure it's right`  
D.93
D.94
D.95  `# Grabs the valence energy from the .lpt file and stores it`  
D.96  `if len(ele) == 2:`  
D.97  `  filename = ele.lower()+str(A)+"y.lpt"`
D.98  `if len(ele) == 1:`  
D.99  `  filename = ele.lower()+"y"+str(A)+"y.lpt"`
D.100  `batfile = open(filename, 'r')`  
D.101  `batfile = batfile.readlines()`  
D.102  `batfile = batfile[5:]`
D.103  `valencestate = 0`
D.104  `for line in batfile:`  
D.105  `  if line[31] == '0' and line[41] == '1':`
D.106  `    valencestate = float(line[13:23].replace(" ",""))`
D.107  `    break`
D.108
D.109  `# Adds the two energies together and prints to a file`  
D.110  `print(valencestate)  # Sanity check to make sure it's right`  
D.111  `bindingenergy = boundstate + valencestate`
D.112  `print(bindingenergy)  # Another sanity check`  
D.113
D.114  `# Saves the total binding energy to file`  
D.115  `stringtoprint = str(A)+'\t'+str(ele)+'\t'+str(E)+'\t'+str(bindingenergy)+'\n'`
D.116
D.117  `if interaction == 'N2LOsat' and VS == '0hw-shell':`
D.118  writeFile = open("././BindingEnergies"+str(A)+"_N2LOsat.txt", 'a+')
D.119
D.120  # For EM1.8/2.0 with 0hw valence space decoupling
D.121  if interaction == 'EM1.8_2.0' and VS == '0hw-shell':
D.122  writeFile = open("././BindingEnergies"+str(A)+"_IMSRG.txt", 'a+')
D.123
D.124  # For EM1.8/2.0 with p, sd, fp valence space decoupling
D.125  if interaction == 'EM1.8_2.0' and VS != '0hw-shell':
D.126  writeFile = open("././SD_Binding_EM.txt", "a+")
D.127
D.128  # For N2LOsat with p, sd, fp valence space decoupling
D.129  if interaction == 'N2LOsat' and VS != '0hw-shell':
D.130  writeFile = open("././SD_Binding_N2.txt", "a+")
D.131
D.132  writeFile.write(stringtoprint)
D.133
D.134  # Return to imsrg directory for another run
D.135  os.chdir("./")
D.136  os.system("pwd")  # Sanity check
D.137  os.chdir("~/imsrg/work/scripts")
D.138
D.139  stop = timeit.default_timer()
D.140  print(stop−start)
Table E.1: Experimental mass excesses taken from [123] except for $^{22}\text{Na}$ and $^{22}\text{Mg}$ which were taken from [42]. Excitation energies and ground state spin-parities taken from [21].

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Table E.1: Continued.

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APPENDIX F
MASS EXCESS CONVERGENCE PLOTS

Mass Excess Convergence for \( A = 10 \)

\( ^{10}\text{Be} \)  \( ^{10}\text{B} \)  \( ^{10}\text{C} \)

Mass Excess Convergence for \( A = 14 \)

\( ^{14}\text{C} \)  \( ^{14}\text{N} \)  \( ^{14}\text{O} \)

Mass Excess Convergence for \( A = 18 \)

\( ^{18}\text{O} \)  \( ^{18}\text{F} \)  \( ^{18}\text{Ne} \)
Mass Excess Convergence for $A = 58$

Mass Excess Convergence for $A = 62$

Mass Excess Convergence for $A = 66$
Mass Excess Convergence for \( A = 70 \)

- \(^{70}\text{Se}\)
- \(^{70}\text{Br}\)
- \(^{70}\text{Kr}\)

Mass Excess Convergence for \( A = 74 \)

- \(^{74}\text{Kr}\)
- \(^{74}\text{Rb}\)
- \(^{74}\text{Sr}\)
APPENDIX G

COULOMB ENERGY OF A UNIFORMLY CHARGED SPHERE

The Coulomb electrostatic energy can be calculated by considering moving infinitesimal charges towards the centre of the sphere from infinity until the entire sphere is complete. This allows the work done on an infinitesimal particle to be written as

\[ dW = \frac{1}{4\pi \varepsilon_0} dq \]

where \( q \) is the total charge of the sphere when the infinitesimal piece of charge \( dq \) is being brought from infinity. For the problem of the uniformly charged sphere, the charge can be given as

\[ q = \rho \frac{4}{3} \pi r^3 \]  \hspace{1cm} (G.2)

as it is a uniform distribution of charge through the volume of a sphere. This gives the infinitesimal charge, as a function of radius, as

\[ dq = \rho 4\pi r^2 dr. \]  \hspace{1cm} (G.3)

Combining Eqs. G.1, G.2, and G.3, the total work done to create the uniformly charged sphere, which is the same as the electrostatic energy, can be written as

\[ W = \int_0^R \frac{4\pi}{3\varepsilon_0} \rho^2 r^4 dr = \frac{4\pi}{15\varepsilon_0} \rho^2 R^5, \]  \hspace{1cm} (G.4)

and rearranging Eq. G.2 gives the density as a function of total charge

\[ \rho = \frac{q}{\frac{4}{3} \pi R^3}. \]  \hspace{1cm} (G.5)

This leads to the form of the total work of

\[ W = \frac{3}{5} \frac{1}{4\pi \varepsilon_0} \frac{q^2}{R}, \]  \hspace{1cm} (G.6)
where the $\frac{1}{4\pi \epsilon_0}$ was left separately so it can be easily converted to units more appropriate for this Thesis. Making the substitutions

\begin{align*}
4\pi \epsilon_0 &= \frac{e^2}{\alpha \hbar c} \\
q &= Ze \\
R &= r_0A^{1/3}
\end{align*}

where $\alpha$ is the fine structure constant ($\alpha \approx \frac{1}{137}$), the work can be rewritten as

\begin{align*}
W &= \frac{3}{5} Z^2 \frac{\alpha \hbar c}{r_0 A^{1/3}}.
\end{align*}
APPENDIX H

ENERGY OF A SPHERE WITH A WOODS SAXON CHARGE DENSITY

Similar to the uniformly charged sphere calculation shown in Appendix G, the potential of a sphere with a Woods Saxon (WS) charge density can be calculated by adding infinitesimally thin sheets of charge to the centre of a sphere until all charge has been added. The work done by adding one infinitesimal sheet as

\[ dW = \frac{1}{4\pi\epsilon_0} \frac{1}{r} q dq, \]  

(H.1)

where \( q \) is the total charge and \( dq \) is the shell. With the WS potential density

\[ \rho(r) = \frac{\rho_0}{1 + e^{\frac{r-R}{a}}} \]  

(H.2)

where \( R \) is the radius of the sphere, the total charge contained in the sphere up to a given radius \( r \) before the addition of another layer is given as

\[ q(r) = \int_0^r 4\pi\tilde{r}^2\rho(\tilde{r})d\tilde{r}, \]  

(H.3)

where \( \tilde{r} \) is a variable of integration. The infinitesimal charge being added, \( dq \), can be found as the charge of a spherical shell at radius \( r \),

\[ dq(r) = 4\pi r^2 \rho(r) dr, \]  

(H.4)

leaving the final equation to solve for the potential of a charged sphere with a WS charge distribution as

\[ W = \frac{1}{4\pi\epsilon_0} \int_0^\infty \left( 4\pi r \rho(r) \int_0^r 4\pi\tilde{r}^2 \rho(\tilde{r})d\tilde{r} \right) dr. \]  

(H.5)

This calculation is done numerically using the code below, which also takes these energies and calculates IMME coefficients from them.
This code is set up to calculate the potential energy of a sphere with a Woods–Saxon charge density. This potential is then used as a binding energy for the calculation of mass excess, which is in turn used to calculate the IMME coefficients for an isobaric analogue triplet.

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Matthew S. Martin
Colorado School of Mines, 2019

---

# Imports packages relevant

```python
import numpy as np
from sys import argv
import matplotlib.pyplot as plt
```

# Constants

```python
mN = 939.5654133; # mass of neutron in MeV
mH = 938.7830583; # mass of hydrogen in MeV
amuFac = 9.314940954e8; # conversion between MeV and amu
```

# Element list

```python
```

# Function for converting binding energy to mass excess

```python
def convert(binding, z, n):
    mass = (binding + z*mH + n*mN) * 1e6 # calculates mass in eV
    massA = mass/amuFac # converts from MeV to amu
    DmK = massA - (n+z) # subtracts A to make it a mass excess
    return (DmK)
```

# Function for calculating IMME B and C Coefficients

```python
def calculateIMME(T1, T0, Tm1):
    b = 0.5*(float(T1)-float(Tm1))
    c = 0.5*(float(T1)+float(Tm1)-2*float(T0))
    return (b, c)
```
# Function for the un-normalized potential

def rho(r):
    rho = 1 / (1 + np.exp((r-R)/a))
    return(rho)

# Function for actually calculating energy

def energy(Z):
    # Creates an evenly spaced array of positions
    blocks = np.linspace(1e-4, largeR, steps)
    # Calculates stepsize
    stepsize = blocks[1] - blocks[0]
    # Creates another array for rho(r), un-normalized
    rhovals = rho(blacks)
    # Sqrt of total charge (QQ exists in function)
    Q = Z * np.sqrt(e)
    # Normalization coefficient for rho(r)
    norm = Q / np.sum(4*np.pi * blocks**2 * rhovals * stepsize)
    # Normalizes rho(r)
    rhovals *= norm
    # Sanity check for rho(r) to make sure it looks right
    plt.plot(blocks, 4*np.pi/3 * rhovals, '-r')
    # Creates the inner integrand
    q_integrands = 4*np.pi * blocks**2 * rhovals
    # Does the inner integral
    q_integrals = np.cumsum(q_integrands) * stepsize
    # Creates the outer integrand
    energy_integrands = 4*np.pi * blocks * rhovals * q_integrals
    # Does the outer integral
    energy = np.sum(energy_integrands) * stepsize
    return(energy)

# Parameters for integral
e = 1.44
eps0 = 1 / (4 * np.pi)
a = 0.524
steps = 50000

Alist = [10,14,18,22,26,30,34,38,42,46,50,54,58,62,66,70,74]
bcoeffs = [0,0,0,0,0,0,0,0,0,0,0,0,0,0,0]
ccoeffs = [0,0,0,0,0,0,0,0,0,0,0,0,0,0,0]
i=0

# Loops through elements and calculates IMME B and C for each
for A in Alist:
    # Sets the Z values to be centred at A/2
H.89  \[ Z_1 = \left(\frac{A}{2}\right) - 1 \]
H.90  \[ N_1 = A - Z_1 \]
H.91  \[ Z_2 = \left(\frac{A}{2}\right) \]
H.92  \[ N_2 = A - Z_2 \]
H.93  \[ Z_3 = \left(\frac{A}{2}\right) + 1 \]
H.94  \[ N_3 = A - Z_3 \]
H.95  \# Sets radius
H.96  \[ R = 1.2 \ast A^{(1/3)} \]
H.97  \# Sets large radius to be 3R so all charge is contained
H.98  \[ \text{largeR} = 3 \ast R \]
H.99  \# Actually does the IMME coefficient calculation
H.100  \[ \text{bcoeffs}[i], \text{ccoeffs}[i] = \text{calculateIMME(convert(energy(Z1), Z1, N1),} \]
        \[ \text{convert(energy(Z2), Z2, N2), convert(energy(Z3), Z3, N3))} \]
H.101  \[ i = i + 1 \]
H.102  
H.103  \# Prints IMME coefficients to be read
H.104  \text{print(bcoeffs)}
H.105  \text{print(cccoeffs)}
APPENDIX I

IMME B COEFFICIENT PLOTS

IMME B Coefficients for \( A = 10 \)

IMME B Coefficients for \( A = 14 \)

IMME B Coefficients for \( A = 18 \)

IMME B Coefficients for \( A = 22 \)

IMME B Coefficients for \( A = 26 \)

IMME B Coefficients for \( A = 30 \)
IMME B Coefficients for $A = 34$

IMME B Coefficients for $A = 38$

IMME B Coefficients for $A = 42$

IMME B Coefficients for $A = 46$

IMME B Coefficients for $A = 50$

IMME B Coefficients for $A = 54$
APPENDIX J

IMME C COEFFICIENT PLOTS
IMME C Coefficients for $A = 58$

IMME C Coefficients for $A = 62$

IMME C Coefficients for $A = 66$

IMME C Coefficients for $A = 70$

IMME C Coefficients for $A = 74$
REFERENCES CITED


[22] National Nuclear Data Center LOGFT Calculator (NNDC), nnDC.bnl.gov/LOGFT/.


