Ab Initio Theory For Two-Neutrino and Neutrinoless Double-Beta Decay

by

Charlie G. Payne

B.Sc., The University of Waterloo, 2015

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF
THE REQUIREMENTS FOR THE DEGREE OF

Master of Science

in

THE FACULTY OF GRADUATE AND POSTDOCTORAL STUDIES

(Physics)

The University of British Columbia
(Waterloo)
(Vancouver)
January 2018

© Charlie G. Payne, 2018
Abstract

Although the complexity behind nuclear physics problems is often deemed too intensive even for modern supercomputers, non-perturbative ab initio (meaning “from first principles”) many-body technologies have made significant strides towards efficiently modelling low-energy QCD structure. In particular, the similarity renormalization group, along with an “in-medium” reference state normal ordering (IM-SRG), has proven useful for making nuclear problems computationally manageable. This IM-SRG method translates chiral Hamiltonians, nuclear properties, and decays into a numerically tractable framework, whilst capturing bulk effects of forces via normal ordering.

A decay that has generated much interest in the nuclear community is double-beta decay. The two-neutrino mode has evaded a proper theoretical treatment, due to a disconcerting puzzle known as “quenching.” The neutrinoless mode (though still hypothetical) could unveil fundamental properties of the neutrino, such as its absolute mass and potential Majorana nature. In this dissertation, we will use IM-SRG, in a valence space shell model construction, to compute both the two-neutrino and neutrinoless double-beta decay of the doubly magic nucleus, Calcium-48.

We conclude that the use of a fully ab initio method that models many-body effects, via IM-SRG, have decreased the two-neutrino double-beta decay nuclear matrix element by a factor of 3 (without any quenching factor), and the neutrinoless counterpart by roughly 20%, compared to the standard phenomenology for Calcium-48. This result has concerning experimental implications, since the half-life of a decay is proportional to the square of the inverse of the nuclear matrix element.
Lay Summary

At the centre of the atom lies a collection of protons and neutrons, bound together in what’s known as the atomic “nucleus.” Although the nucleus represents one of the most fundamental building blocks of matter, and therefore of reality itself, its structure is still mysterious in the context of theoretical physics. In particular, using many-body quantum mechanics to predict how the nucleus might decay and emit elementary particles is of primary interest to theorists and experimentalists alike. One of these decays, which we focus on in this dissertation, is called “double-beta decay;” and it has generated much excitement in the community due to its potential to unveil the secrets of the most elusive elementary particle: the neutrino. By studying the nuclear structure of Calcium-48, and its ability to double-beta decay, we attempt to set bounds on the mass of the neutrino.
Preface

This dissertation is original, unpublished work by the author, C. G. Payne. The software imsrg++ and nutbar, developed by Dr. Ragnar Stroberg at TRIUMF [1, 2], and the shell model code NuShellX, developed by Alex Brown at Michigan State University [3] and Bill Rae from Garisgonton, Oxfordshire [4], were used to obtain the results of this dissertation, as described in Chapter 6. Dr. Stroberg was the post-doctoral collaborator of the author’s research supervisor at TRIUMF, Dr. Jason D. Holt. Together, the author, Dr. Holt, and Dr. Stroberg plan to publish refined results on Calcium-48 in collaboration with Dr. Gaute Hagen,∗ et al, whom use the coupled cluster many-body method. Additionally, work on Germanium-76 is expected to be published in collaboration with Dr. Javier Menéndez.† Benchmarking of the neutrinoless double-beta decay matrix elements (see Chapter 4) was aided by Dr. Jonathan Engel.‡ Appendices A, B, and C are based on the textbook “From Nucleons to Nucleus: Concepts of Microscopic Nuclear Theory” by J. Suhonen [5] for introductory purposes.

*Oak Ridge National Laboratory
†University of Tokyo
‡University of Northern Carolina, Chapel Hill
# Table of Contents

Abstract ............................................................................. ii

Lay Summary ................................................................. iii

Preface .............................................................................. iv

Table of Contents ........................................................... v

List of Tables ....................................................................... viii

List of Figures ...................................................................... ix

List of Acronyms ............................................................. x

Acknowledgements ........................................................... xii

Dedication ......................................................................... xiii

1 Introduction ...................................................................... 1

2 Preliminaries .................................................................... 2
  2.1 Many-Body Quantum Mechanics ................................. 2
      2.1.1 Central Quantum Harmonic Oscillator ............... 2
      2.1.2 The Talmi-Moshinsky Transformation ............... 4
      2.1.3 Slater Determinants and the Pauli Exclusion Principle 7
      2.1.4 The Hartree-Fock Method ................................. 8
  2.2 Nuclear Structure Theory ........................................... 9
      2.2.1 The Basics ...................................................... 9
      2.2.2 Nuclear Shell Model ...................................... 11
      2.2.3 Nuclear Interactions ...................................... 12
      2.2.4 Nuclear Many-Body Methods ............................. 14
  2.3 Beta Decay .................................................................. 15
      2.3.1 Parity Violation .............................................. 15
      2.3.2 Allowed Fermi Transition ............................... 16
      2.3.3 Allowed Gamow-Teller Transition .................... 16
# Table of Contents

2.3.4 Quenching in Single-Beta Decay ........................................... 18

3 Double-Beta Decay ................................................................. 19
  3.1 Two-Neutrino Double-Beta Decay .............................................. 19
    3.1.1 Experimental Confirmation of $2\nu\beta\beta$ ......................... 20
    3.1.2 $2\nu\beta\beta$ Half-Life Formula ...................................... 21
    3.1.3 $M^{2\nu}$ Matrix Elements ............................................. 23
    3.1.4 Quenching in $2\nu\beta\beta$ ........................................... 25
  3.2 From Two Neutrinos to None .................................................. 25
  3.3 Neutrinoless Double-Beta Decay ............................................. 31
    3.3.1 Current Experimental Status for $0\nu\beta\beta$ ....................... 31
    3.3.2 $0\nu\beta\beta$ Half-Life Formula ...................................... 32
    3.3.3 Nuclear Matrix Elements ............................................... 34
    3.3.4 The Closure Approximation ............................................ 35

4 $M^{0\nu}$ Two-Body Matrix Elements ........................................... 36
  4.1 Deconstructing $M^{0\nu}$ ................................................... 36
  4.2 Tensor TBMEs ................................................................. 39
  4.3 Gamow-Teller TBMEs ......................................................... 42
  4.4 Fermi TBMEs ................................................................. 44
  4.5 Relative Bessel’s Matrix Elements ....................................... 45
    4.5.1 RBMEs with Short-Range Correlations ................................ 48
  4.6 Reconstructing $M^{0\nu}$ TBMEs ........................................... 49

5 Valence Space In-Medium Similarity Renormalization Group ............... 53
  5.1 Nuclear Core and Valence Space ........................................... 53
    5.1.1 Model Space ............................................................ 54
  5.2 Similarity Renormalization Group ......................................... 55
    5.2.1 Nuclear Potentials and Similarity Transformations .................. 56
    5.2.2 SRG Flow Equations .................................................... 57
    5.2.3 Consistent Operator Evolution ....................................... 59
  5.3 Reference State Normal Ordering ......................................... 60
    5.3.1 Hartree-Fock Step ....................................................... 61
  5.4 The Magnus Formulation ..................................................... 61

6 Numerical Methods ............................................................... 64
  6.1 imsr++ ................................................................................. 64
  6.2 NuShellX@MSU ....................................................................... 65
  6.3 nutbar .................................................................................. 65
  6.4 Two-Tiered Adaptive $M^{0\nu}$ TBMEs ....................................... 65
    6.4.1 Integration Techniques from GSL ....................................... 67
# Table of Contents

7 Results ................................................. 68
  7.1 $2\nu\beta\beta$ NME for $^{48}\text{Ca}$ ....................... 68
     7.1.1 Phenomenological Benchmarking ..................... 69
     7.1.2 VS-IM-SRG Using the EM 1.8/2.0 Interaction .......... 71
  7.2 $0\nu\beta\beta$ NME for $^{48}\text{Ca}$ ....................... 72
     7.2.1 Phenomenological Benchmarking ..................... 73
     7.2.2 VS-IM-SRG Using the EM 1.8/2.0 Interaction .......... 75
     7.2.3 VS-IM-SRG Using the 500/400 $N^3\text{LO}+3\text{N}$ Interaction ....... 77
     7.2.4 Summary ..................................... 77

8 Conclusions ........................................... 81

Bibliography ........................................... 82

Appendix A Angular Momentum Coupling .......................... 95
  A.1 Clebsch-Gordan Coefficients .......................... 95
  A.2 The Wigner 3$j$-Symbols ............................ 99
  A.3 Coupling Three Angular Momenta ..................... 100
  A.4 Coupling Four Angular Momenta ..................... 101

Appendix B Spherical Tensor Operators .......................... 103
  B.1 Definitions ..................................... 103
  B.2 Reduced Matrix Elements ........................... 106
  B.3 The Wigner-Eckart Theorem .......................... 106
  B.4 Decomposition Theorems ............................ 108

Appendix C Fock Space and Operators .......................... 114
  C.1 Normal Ordering and Contractions ................... 115
    C.1.1 Wick’s Theorem .................................. 116
  C.2 One-Body Operators ................................ 117
  C.3 Two-Body Operators ................................ 119
    C.3.1 The Closure Approximation ...................... 121

Appendix D Summation Limits for the Talmi-Moshinsky Transformation .. 122

Appendix E Derivation of Equation (D11) from PRC.88.064312(2013) ...... 126

Appendix F Miscellaneous Formulae .......................... 129
List of Tables

<table>
<thead>
<tr>
<th>Table 4.1:</th>
<th>Common SRC parameters for the Jastrow-type function</th>
<th>48</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 6.1:</td>
<td>Two-tiered integration scheme for $M^{0\nu}$ TBMEs</td>
<td>66</td>
</tr>
<tr>
<td>Table 7.1:</td>
<td>Values of $M^{0\nu}$ parameters</td>
<td>73</td>
</tr>
<tr>
<td>Table 7.2:</td>
<td>Benchmarking for the neutrinoless double-beta decay NME of $^{48}$Ca using a $pf$-shell valence space and the GXPF1A interaction</td>
<td>74</td>
</tr>
<tr>
<td>Table 7.3:</td>
<td>Comparison of the neutrinoless double-beta decay NMEs, for benchmarking</td>
<td>75</td>
</tr>
<tr>
<td>Table 7.4:</td>
<td>Summary of the VS-IM-SRG evolved neutrinoless double-beta decay NMEs of $^{48}$Ca using a $pf$-shell valence space</td>
<td>77</td>
</tr>
</tbody>
</table>
## List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Oxygen-16, as represented by the nuclear shell model</td>
<td>12</td>
</tr>
<tr>
<td>2.2</td>
<td>Hierarchy of nuclear forces in $\chi$EFT</td>
<td>14</td>
</tr>
<tr>
<td>3.1</td>
<td>The nuclear Feynman diagram for double-beta decay</td>
<td>20</td>
</tr>
<tr>
<td>3.2</td>
<td>Even and odd mass parabolas of $A = 48$ isobars</td>
<td>21</td>
</tr>
<tr>
<td>3.3</td>
<td>The nuclear Feynman diagram for neutrinoless double-beta decay</td>
<td>26</td>
</tr>
<tr>
<td>3.4</td>
<td>The nuclear Feynman diagram for $0\nu\beta\beta$ via a pion exchange</td>
<td>28</td>
</tr>
<tr>
<td>3.5</td>
<td>Reconstructing the blackbox theorem of Schechter and Valle</td>
<td>30</td>
</tr>
<tr>
<td>5.1</td>
<td>Core, valence space, and excluded region for the ground state of $^{48}$Ca</td>
<td>54</td>
</tr>
<tr>
<td></td>
<td>within the nuclear shell model</td>
<td></td>
</tr>
<tr>
<td>7.1</td>
<td>Benchmarking for the two-neutrino double-beta decay NME of $^{48}$Ca</td>
<td>70</td>
</tr>
<tr>
<td></td>
<td>using a $pf$-shell valence space and the GXPF1A interaction</td>
<td></td>
</tr>
<tr>
<td>7.2</td>
<td>VS-IM-SRG evolved two-neutrino double-beta decay NME of $^{48}$Ca</td>
<td>71</td>
</tr>
<tr>
<td></td>
<td>using a $pf$-shell valence space and the EM 1.8/2.0 interaction</td>
<td></td>
</tr>
<tr>
<td>7.3</td>
<td>VS-IM-SRG evolved neutrinoless double-beta decay NME of $^{48}$Ca</td>
<td>78</td>
</tr>
<tr>
<td></td>
<td>using a $pf$-shell valence space and the EM 1.8/2.0 interaction</td>
<td></td>
</tr>
<tr>
<td>7.4</td>
<td>VS-IM-SRG evolved neutrinoless double-beta decay NME of $^{48}$Ca</td>
<td>79</td>
</tr>
<tr>
<td></td>
<td>using a $pf$-shell valence space and the EM 1.8/2.0 interaction, including</td>
<td></td>
</tr>
<tr>
<td></td>
<td>AV18 short-range correlations</td>
<td></td>
</tr>
<tr>
<td>7.5</td>
<td>VS-IM-SRG evolved neutrinoless double-beta decay NME of $^{48}$Ca</td>
<td>80</td>
</tr>
<tr>
<td></td>
<td>using a $pf$-shell valence space and the 500/400 N$^3$LO+3N interaction</td>
<td></td>
</tr>
</tbody>
</table>
# List of Acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>χEFT</td>
<td>Chiral Effective Field Theory</td>
</tr>
<tr>
<td>0νββ</td>
<td>neutrinoless double-beta (decay)</td>
</tr>
<tr>
<td>2νββ</td>
<td>two-neutrino double-beta (decay)</td>
</tr>
<tr>
<td>2N, 3N, ...</td>
<td>Two-Nucleon, Three-Nucleon, ...</td>
</tr>
<tr>
<td>amu</td>
<td>(unified) atomic mass unit</td>
</tr>
<tr>
<td>BCH</td>
<td>Baker-Cambell-Hausdorff</td>
</tr>
<tr>
<td>BSM</td>
<td>Beyond (the) Standard Model</td>
</tr>
<tr>
<td>CG</td>
<td>Clebsch-Gordan</td>
</tr>
<tr>
<td>CKM</td>
<td>Cabibbo-Kobayashi-Maskawa</td>
</tr>
<tr>
<td>CoM</td>
<td>Centre of Mass</td>
</tr>
<tr>
<td>CTML</td>
<td>Chosen Talmi-Moshinsky Limits</td>
</tr>
<tr>
<td>F</td>
<td>Fermi</td>
</tr>
<tr>
<td>g.s.</td>
<td>ground state</td>
</tr>
<tr>
<td>GT</td>
<td>Gamow-Teller</td>
</tr>
<tr>
<td>h.c.</td>
<td>hermitian conjugate</td>
</tr>
<tr>
<td>IM-SRG</td>
<td>In-Medium Similarity Renormalization Group</td>
</tr>
<tr>
<td>LECs</td>
<td>Low-Energy Coupling Constants</td>
</tr>
<tr>
<td>LHS</td>
<td>Left Hand Side</td>
</tr>
<tr>
<td>LNV</td>
<td>Lepton Number Violation (or Violating)</td>
</tr>
<tr>
<td>MEC</td>
<td>Meson Exchange Current</td>
</tr>
<tr>
<td>NLO, N^2LO, ...</td>
<td>Next-to-Leading Order, Next-to-Next-to-Leading Order, ...</td>
</tr>
<tr>
<td>NME</td>
<td>Nuclear Matrix Element</td>
</tr>
<tr>
<td>OBMEs</td>
<td>One-Body Matrix Elements</td>
</tr>
<tr>
<td>OBTDs</td>
<td>One-Body Transition Densities</td>
</tr>
<tr>
<td>ODE</td>
<td>Ordinary Differential Equation</td>
</tr>
<tr>
<td>o.w.</td>
<td>otherwise</td>
</tr>
<tr>
<td>Acronym</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>--------------------------------------</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial Differential Equation</td>
</tr>
<tr>
<td>PMNS</td>
<td>Pontecorvo-Maki-Nakagawa-Sakata</td>
</tr>
<tr>
<td>QCD</td>
<td>Quantum Chromodynamics</td>
</tr>
<tr>
<td>QFT</td>
<td>Quantum Field Theory</td>
</tr>
<tr>
<td>QHO</td>
<td>Quantum Harmonic Oscillator</td>
</tr>
<tr>
<td>RBMEs</td>
<td>Relative Bessel’s Matrix Elements</td>
</tr>
<tr>
<td>RHS</td>
<td>Right Hand Side</td>
</tr>
<tr>
<td>ShM</td>
<td>(Nuclear) Shell Model</td>
</tr>
<tr>
<td>SRCs</td>
<td>Short-Range Correlations</td>
</tr>
<tr>
<td>SRG</td>
<td>Similarity Renormalization Group</td>
</tr>
<tr>
<td>T</td>
<td>Tensor</td>
</tr>
<tr>
<td>TBMEs</td>
<td>Two-Body Matrix Elements</td>
</tr>
<tr>
<td>TBTDs</td>
<td>Two-Body Transition Densities</td>
</tr>
<tr>
<td>TISE</td>
<td>Time-Independent Schrödiner Equation</td>
</tr>
<tr>
<td>VS</td>
<td>Valence Space</td>
</tr>
<tr>
<td>WLOG</td>
<td>Without Loss of Generality</td>
</tr>
</tbody>
</table>
Acknowledgements

Of foremost importance, I would like to thank my research supervisor, Dr. Jason D. Holt, for taking me on as a M.Sc. student and guiding me through this challenging project. He gave me the chance to tackle nuclear physics, a field which I had no prior experience in. Abundant thanks go to Dr. Ragnar Stroberg, our post-doctoral collaborator, for motivating this research and providing me with steadfast assistance. During the course of my work, we had several co-op students in our small team, who provided input: David Livermore, Oliver Drozdowski, Samuel Leutheusser, and Chan Gwak.

Many thanks are in order for TRIUMF, its facilities, and all its employees - in particular those at the theory department. TRIUMF has been a truly wonderful experience. As a theory student, being so close to experiment and phenomenology helps to keep you grounded in reality, instead of becoming lost in abstraction. Lively discussions with all the students at the office, past and present, kept me sane. My sincere gratitude goes to Prof. Reiner Kruecken, the current Deputy Director of TRIUMF, who acted as my academic supervisor.

I would also like to thank Prof. Jon Engel, Dr. Javier Menéndez, Dr. Gaute Hagen, Dr. Mirko Miorelli, and Javier Hernandez, for their fruitful insight into components of this research.

Special thanks go to my parents, Joe Payne and Pam Hudson, and my sister, Melissa Hudson. My family have always cheered on my progress and supported me through the worst of times, and without them this thesis would not have been possible.
In loving memory of Umpa, Rob, and Gracey
Chapter 1

Introduction

Despite being extraordinarily unintuitive, quantum mechanics, in its many-body formulation, describes physics from solid state devices, all the way to the hadronization of jets in high-energy supercolliders. At lower energies, like those on the scale of the atomic nucleus, quantum many-body theory is currently undergoing a foundational refurbishment [6]. Theorists are migrating from phenomenological models to new technologies built from first principles (ab initio). This requires taking realistic nuclear interactions, like those derived from chiral effective field theory [7], and combining them with novel many-body methods to make predictions of nuclear observables. Such a daunting task has, historically, proven to be notoriously computationally intensive [8]. Thus, nuclear structure theorists are focused on making the nuclear problem more numerically tractable, whilst also capturing all the relevant higher-order phenomena.

One missing piece that has been neglected by nuclear theorists is the inclusion of three-nucleon forces - until recently [9–11]. By using a redefined notion of normal ordering, the in-medium similarity renormalization group can capture three-nucleon interactions and consistently incorporate them into operators other than just the Hamiltonian [12]. Furthermore, by decoupling a nucleonic valence space with the SRG, diagonalization is made more efficient. With this method in place, an intriguing question is: how do these three-nucleon interactions, embedded into nuclear structure theory, affect nuclear properties and decays? A nuclear decay of primary interest is double-beta decay, with its neutrinoless mode as an exciting prospect due to the discovery of neutrino oscillations [13, 14]. Before that can be approached, one hopes that the problem of “quenching” (see Section 3.1.4) in two-neutrino double-beta decay can be solved using nuclear structure theory. We will attempt to model both of these decays using the so-called Magnus formulation of IM-SRG for the medium-mass nucleus, Calcium-48.

This dissertation is organized as follows. First, in Chapter 2, we will outline the preliminary content needed to develop nuclear many-body theory and the fundamentals behind double-beta decay, while making frequent reference to introductory material in Appendices A, B, and C. After overviewing the status of double-beta decay in Chapter 3, we’ll do a rigorous derivation of the neutrinoless double-beta decay two-body matrix elements in Chapter 4. To model this decay ab initio, we use the valence space formulation of IM-SRG, which we describe in detail in Chapter 5. Finally, after outlining our numerical methods in Chapter 6, we’ll conclude with the results of computations for Calcium-48 in Chapter 7.

*Neutrino oscillations prove that (at least one) neutrino has a non-zero mass, which is a necessary (but not sufficient) requirement for the theory behind neutrinoless double-beta decay (see Section 3.2).
†Calcium-48 is a doubly magic nucleus, making it an ideal benchmark for our theoretical framework.
Chapter 2

Preliminaries

Before we can present the main work of this dissertation, it is essential to lay out the mathematical framework for nuclear physics. This chapter will help give unfamiliar readers an overview of the techniques we use, and also to establish the notation we’ll be using throughout the course of this dissertation. Any readers who find themselves uncomfortable with the theoretical machinery of this chapter should first read: Appendices A, B, and C. The prescriptions laid out in [5, 15, 16] will be closely followed. We’ll assume the reader has a background in: quantum mechanics, statistical mechanics, Lagrangian and Hamiltonian dynamics, particle physics of the Standard Model, some quantum field theory (QFT), linear algebra over complex vector spaces, multivariate calculus, vector calculus, ordinary differential equations (ODEs), partial differential equations (PDEs), complex analysis, numerical methods, and some group theory.

2.1 Many-Body Quantum Mechanics

Let’s begin by bridging the gap between the abstractions of Appendices A, B, and C and the coveted nuclear landscape. Since the atomic nucleus is a collection of bound nucleons (protons and neutrons) interacting through the strong nuclear force, many-body quantum mechanics will be the path to nuclear structure theory.

2.1.1 Central Quantum Harmonic Oscillator

In nuclear physics, the solutions to the Time-Independent Schrödinger Equation (TISE) under a spherically symmetric central potential are often used as a starting point, which is referred to as the “(harmonic) oscillator basis.” Specifically, under the central potential

\[ V(r) = \frac{1}{2} m_N \omega^2 r^2 - V_0 \]

where \( \omega \), or \( \hbar \omega \) [MeV], is the “(oscillator) frequency,” \( m_N \) is the mass of a nucleon, and \( V_0 \) comes from an experimental fit - the radial TISE becomes

\[ -\frac{\hbar^2}{2m_N} \left[ \nabla_r^2 - \frac{l(l+1)}{2} \right] R_{nl}(r) - V_0 + \frac{1}{2} m_N \omega^2 r^2 R_{nl}(r) = E_{nl} R_{nl}(r) \tag{2.1} \]

This equation can be thought of as describing a nucleon oscillating about a central effective core* with the total wave-function

*or simply another nucleon in relative coordinates
2.1. Many-Body Quantum Mechanics

\[ \Psi_{nlm}(\vec{r}, t) = \psi_{nlm}(\vec{r})T_{nl}(t) = R_{nl}(r)Y_{lm}(\theta, \phi)e^{-\frac{i}{\hbar}E_{nl}t} \]

where \( R_{nl}(r) \) is the (relative) radial wave-function, \( Y_{lm}(\theta, \phi) \) are your standard spherical harmonics* as in Equation (F7), \( nlm \) are the three necessary quantum numbers as per usual, and the quantized energy levels are

\[ E_{nl} = \left( N + \frac{3}{2} \right) \hbar \omega - V_0, \quad N \equiv 2n + l \] (2.2)

As with common convention, we’ll label the principle quantum number, \( n = 0, 1, 2, ... \), as counting the number of nodes of the radial wave-function. It can be shown [17] that the solution to Equation (2.1) is

\[ R_{nl}(r) = N_{nl} \left( \frac{r}{b} \right)^l e^{-\frac{r^2}{2b^2}} L_n^{l+\frac{1}{2}}(r^2/b^2) \] (2.3)

where \( b \) is the “(harmonic) oscillator length,” given by

\[ b \equiv \sqrt{\frac{\hbar}{m_N \omega}} \approx \frac{197.3269788}{\sqrt{938.9187474 \times \hbar \omega [\text{MeV}]}} \text{ fm} \] (2.4)

Here we have taken our numerical values from CODATA-2014 [18], and set the nucleon mass as the average of the proton mass and the neutron mass

\[ m_N \equiv \frac{m_p + m_n}{2} = 938.9187474 \text{ MeV} \]

\( N_{nl} \) in Equation (2.3) is the normalization constant, which can be found as

\[ N_{nl} = \sqrt{\frac{2n!}{b^3 \Gamma(n+l+\frac{3}{2})}} \] (2.5)

where \( \Gamma(x) \) is the Gamma function, as in Equation (F1). Finally, the \( L_n^\alpha(x) \) in Equation (2.3) are the generalized Laguerre polynomials with \( \alpha, \beta \in \mathbb{R} \), which are defined as solutions to the frequently reoccurring ODE in physics, Equation (F3).

It’s important to note that the harmonic oscillator wave-functions form a complete basis, which will have much utility in the future

\[ \int_0^\infty R_{nl}(r)R_{n'l}(r)r^2dr = \delta_{nn'} \]

An optimal oscillator frequency can be found from the Blomqvist-Molinari formula of nuclear charge radius predictions, from the well-known paper [19]

\[ \hbar \omega \approx \left( 45A^{-\frac{1}{3}} - 25A^{-\frac{2}{3}} \right) \text{ MeV} \] (2.6)

where, of course, \( A = N + Z \) is the “mass number” of the nucleus of interest, i.e., the sum of the number of constituent neutrons, \( N \), and protons, \( Z \). By sneakily introducing some nuclear parlance, we’ve suggested that the quantum harmonic oscillator (QHO) described above has an inherent relation to nuclear structure. More on this will be explored soon in Section 2.2.2.

*via the angular TISE
2.1. Many-Body Quantum Mechanics

2.1.2 The Talmi-Moshinsky Transformation

Marcos Moshinsky developed a method to transform between two particles in a harmonic oscillator basis to their relative and centre of mass (CoM) coordinates, using work done by Igal Talmi in the early 1950’s [20, 21]. Let’s label the “lab frame” bases as \(|n_i l_i| i = 1, 2\), the relative coordinate basis as \(|n_r l_r\rangle\), and the CoM basis as \(|N\Lambda\rangle\). To stay consistent with the notation throughout this dissertation, the total angular momentum is labelled \(\vec{L}\), so that

\[
\vec{l}_1 + \vec{l}_2 = \vec{L} = \vec{l}_r + \vec{\Lambda} \tag{2.7}
\]

where, if \(\vec{r}_1\) and \(\vec{r}_2\) represent the coordinates of each particle in the lab frame, then the relative coordinates and CoM coordinates are given by

\[
\vec{r} \equiv \frac{1}{\sqrt{2}} (\vec{r}_1 - \vec{r}_2) \quad \text{and} \quad \vec{R} \equiv \frac{1}{\sqrt{2}} (\vec{r}_1 + \vec{r}_2) \tag{2.8}
\]

Take close notice of the inverse factor of square root two in front of these definitions, since it will cause some notational trouble later on.

Just as the basis \(|n_1 l_1, n_2 l_2 : LM\rangle\) is complete, so is \(|n_r l_r, N\Lambda : LM\rangle\), and so we can play the well known trick of inserting an identity into an arbitrary state as so

\[
|n_i l_i, n_j l_j : LM\rangle = \mathbb{1} \cdot |n_i l_i, n_j l_j : LM\rangle = \left(\sum |n_r l_r, N\Lambda : LM\rangle \langle n_r l_r, N\Lambda : LM|\right) |n_i l_i, n_j l_j : LM\rangle
= \sum \langle n_r l_r, N\Lambda : LM|n_i l_i, n_j l_j : LM\rangle |n_r l_r, N\Lambda : LM\rangle
= \sum_{n_r} D_{ij} |n_r l_r, N\Lambda : LM\rangle \tag{2.9}
\]

In Equation (2.9) we’ve slipped in a definition, so let’s make it official:

**Definition 2.1: “Talmi-Moshinsky Brackets”**

The coefficients from Equation (2.9) above are defined as

\[
D_{ij} \equiv \langle n_r l_r, N\Lambda : L|n_i l_i, n_j l_j : L\rangle \tag{2.10}
\]

where we have the couplings \(\Delta(l_i l_j : L)\) and \(\Delta(l_r \Lambda : L)\) from Equation (2.7). Note that in many papers authors will switch the \(\Lambda \leftrightarrow L\), including Moshinsky himself. Also, we’ve dropped the \(M\)-dependence in this definition, since it is well known that the Talmi-Moshinsky brackets are independent of the total orbital angular momentum projection [22]. Finally, the common convention is to take it that

\[
D_{ij} = \langle n_r l_r, N\Lambda : L|n_i l_i, n_j l_j : L\rangle \doteq \langle n_i l_i, n_j l_j : L|n_r l_r, N\Lambda : L\rangle
\]

In other words, like the Clebsch-Gordan (CG) coefficients, these brackets are real, so \(D_{ij} = D_{ij}^*\). These coefficients can be calculated via algorithms given in [23, 24].
A question that appears much less heinous than it actually is, is: in Equation (2.9), what limits does the sum run over? Since this issue gets rather involved, we’ll leave it for Appendix D. For instance, see the chosen Talmi-Moshinsky limits (CTML) given in Equation (D13).

The power of these Talmi-Moshinsky brackets is that they give us a means of doing physics in the relative frame, which will often be more intuitive and convenient than the lab frame. Hence, when calculating two-body reduced matrix elements (see Section C.3), we’ll typically transform from lab frame into relative coordinates via these brackets. This step is important enough that we label it as a theorem:

**Theorem 2.1: “Talmi-Moshinsky Transformation”**

Consider a two-body spherical tensor operator, $\hat{T}$, with rank $R$. We can transform from the lab frame representation to the relative/CoM coordinates using the formula

$$
\langle l_1, l_2 ; L | \hat{T}_R | l'_1, l'_2 ; L' \rangle = \sum_{n_{rL}, n'_r} D_{12} D'_{12} (-1)^{R+L' + l_r + \Lambda} \cdot \langle n_{rL} | n_r | l_1, l_2 ; L \rangle \langle n'_r | n'_r | l'_1, l'_2 ; L' \rangle
$$

where the CTML are given in Equation (D21), and the brackets are

$$
D_{12} = \langle n_r l_r, N\Lambda ; L | n_1 l_1, n_2 l_2 ; L \rangle \quad \text{and} \quad D'_{12} = \langle n'_r l'_r, N'\Lambda' ; L' | n'_1 l'_1, n'_2 l'_2 ; L' \rangle
$$

The utility of this formula cannot be overstated. In essence, we now have a way of transforming two-body matrix elements in the lab frame representation into a sum of one-body matrix elements in the relative coordinate space! Remarkably, all the information involving the CoM frame has been encoded by the Talmi-Moshinsky brackets, the phase factor, and the $6j$-symbol.

**Proof of Theorem (2.1).**

First, let’s transform the states of the matrix elements on the left hand side (LHS) of Equation (2.11) using (2.9), in other words

$$
||l'_1, l'_2 ; L' \rangle = \sum_{n'_r l'_r, N'\Lambda'} \langle n'_r l'_r, N'\Lambda' ; L' | n'_1 l'_1, n'_2 l'_2 ; L' \rangle ||n'_r l'_r, N'\Lambda' ; L' \rangle \quad \text{and},
$$

$$
\langle l_1, l_2 ; L \rangle = \sum_{n_{rL}, n_r} \langle n_1 l_1, n_2 l_2 ; L | n_{rL}, N\Lambda ; L \rangle \langle n_{rL}, N\Lambda ; L \rangle
$$

so take it that

$$
D_{12} \equiv \langle n_1 l_1, n_2 l_2 ; L | n_{rL}, N\Lambda ; L \rangle \quad \text{and} \quad D'_{12} \equiv \langle n'_r l'_r, N'\Lambda' ; L' | n'_1 l'_1, n'_2 l'_2 ; L' \rangle
$$

(2.13)
This gives the reduced matrix elements
\[ \langle l_1, l_2; L|\hat{\mathcal{T}}_R||l'_1, l'_2; L' \rangle = \sum_{n_r \Lambda \Lambda'} \sum_{n'_r \Lambda' \Lambda''} D_{12} D'_{12} \langle n_r l_r, N\Lambda; L|\hat{\mathcal{T}}_R||n'_r l'_r, N'\Lambda'; L' \rangle \] (2.14)

Now, from Proposition B.1 and Equation (B4), we may take it that \( \hat{\mathcal{T}}_R = [\hat{\mathcal{T}}_R \otimes 1_0]_R \), and apply Theorem (B.2) - Equation (B15) to the reduced matrix elements on the right hand side (RHS) of (2.14)

\[ \langle n_r l_r, N\Lambda; L|\hat{\mathcal{T}}_R||n'_r l'_r, N'\Lambda'; L' \rangle = \hat{L} \hat{R} \hat{L}' \begin{pmatrix} l_r & \Lambda & L \\ l'_r & \Lambda' & L' \\ R & 0 & R \end{pmatrix} \langle n_r l_r||\hat{\mathcal{T}}_R||n'_r l'_r \rangle \langle N\Lambda||1||N'\Lambda' \rangle \] (2.15)

We know from the result in Equation (B12) that
\[ \langle N\Lambda||1||N'\Lambda' \rangle = \delta_{NN'}\delta_{\Lambda\Lambda'} \hat{\Lambda} \] (2.16)

and also, from Equations (A38), (A39), and (A28), we can obtain
\[ \begin{pmatrix} l_r & \Lambda & L \\ l'_r & \Lambda' & L' \\ R & 0 & R \end{pmatrix} = \delta_{\Lambda\Lambda'}(-1)^{l_r + l'_r + \Lambda + R} \hat{\Lambda}^{-1} \hat{R}^{-1} \begin{pmatrix} L & l_r & \Lambda \\ l'_r & L' & R \end{pmatrix} \] (2.17)

Plugging Equation (2.16) and (2.17) into (2.15) yields
\[ \langle n_r l_r, N\Lambda; L|\hat{\mathcal{T}}_R||n'_r l'_r, N'\Lambda'; L' \rangle = \delta_{NN'}\delta_{\Lambda\Lambda'}(-1)^{R+L'+l_r + \Lambda} \hat{L} \hat{L}' \begin{pmatrix} L & l_r & \Lambda \\ l'_r & L' & R \end{pmatrix} \langle n_r l_r||\hat{\mathcal{T}}_R||n'_r l'_r \rangle \] (2.18)

And now inserting Equation (2.18) into (2.14) gives
\[ \langle l_1, l_2; L|\hat{\mathcal{T}}_R||l'_1, l'_2; L' \rangle = \hat{L}' \sum_{n_r \Lambda \Lambda'} \sum_{n'_r \Lambda' \Lambda''} \delta_{NN'}\delta_{\Lambda\Lambda'} D_{12} D'_{12} (-1)^{R+L'+l_r + \Lambda} \] (2.19)
\[ \times \begin{pmatrix} L & l_r & \Lambda \\ l'_r & L' & R \end{pmatrix} \langle n_r l_r||\hat{\mathcal{T}}_R||n'_r l'_r \rangle \]

Finally, we may perform the sum over the \( N'\Lambda' \) in Equation (2.19), which will retrieve (2.11), and likewise send \( D'_{12} \rightarrow D_{12} \) from (2.13) to (2.12) respectively.

\( \square \)

**Corollary 2.1.1**

Consider a two-body spherical tensor operator, \( \hat{T} \), with rank 0. We can transform from the lab frame representation to the relative/CoM coordinates using the formula
\[ \langle l_1, l_2; L|\hat{T}||l'_1, l'_2; L' \rangle = \delta_{LL'} \hat{L} \sum_{n_r \Lambda \Lambda'} D_{12} D'_{12} \hat{L}^{-1} \langle n_r l_r||\hat{T}||n'_r l'_r \rangle \] (2.20)

where the CTML are given in Equation (D16), and the brackets are
2.1. Many-Body Quantum Mechanics

\[ D_{12} = \langle n_r l_r, N \Lambda; L | n_1 l_1, n_2 l_2; L \rangle \quad \text{and}\quad D_{12}^{i'j'} = \langle n_r' l_r', N \Lambda; L | n_1' l_1', n_2' l_2'; L \rangle \quad (2.21) \]

The proof of Corollary 2.1.1 above is a straightforward application of Theorem 2.1 and the identity in Equation (A30), where one must keep track of the Kronecker-deltas accordingly, note that \( l_r, \Lambda, L \in \mathbb{N}_0 \), and keep track of the change of notation in the brackets. Another easily proven (but less physically applicable) corollary is given in Equation (F10).

2.1.3 Slater Determinants and the Pauli Exclusion Principle

In single-body quantum mechanics, we describe a particle with a wave-function, which we now label \( \Phi(\vec{r}, t) = \langle \vec{r} | \Phi(t) \rangle \), which satisfies the Schrödiner equation. By doing separation of variables, the corresponding time-independent wave-function will be written as \( \phi(\vec{r}) \). The next natural question is: for \( A \) particles, each tracked in their respective coordinates system by \( \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A \), how would we construct a many-body wave-function?

Definition 2.2: “Slater Determinant”

Let’s presuppose that each fermion in an \( A \)-body system satisfies their own TISE with the normalized wave-function \( \phi_i(\vec{r}_i) \) for \( i = 1, 2, \ldots, A \). Then an ansatz for the many-body wave-function is

\[ \Psi_0(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_1(\vec{r}_1) & \phi_1(\vec{r}_2) & \cdots & \phi_1(\vec{r}_A) \\ \phi_2(\vec{r}_1) & \phi_2(\vec{r}_2) & \cdots & \phi_2(\vec{r}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_A(\vec{r}_1) & \phi_A(\vec{r}_2) & \cdots & \phi_A(\vec{r}_A) \end{vmatrix} \quad (2.22) \]

where the prefactor is to ensure this “Slater determinant” wave-function is, itself, normalized.

Notice that we’ve now inherently switched to describing a collection of fermions, which will be convenient for us since the nucleon is a spin-1/2 particle. The naught subscript on \( \Psi_0 \) is there to distinguish this from the time-dependant many-body wave-function, \( \Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A, t) \). Using the determinant in Definition 2.2 guarantees that this many-body wave-function will be properly anti-symmetrized, in that it will obey the Pauli exclusion principle

\[ \Psi_0(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = (-1)^{\Pi(P)} \Psi_0(P(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A)) \quad (2.23) \]

where \( \Pi(P) \) is the number of interchanges of two coordinates required to bring the permutation \( P \) back to identity. For example, for \( P(\vec{r}_1, \vec{r}_2, \vec{r}_3) = (\vec{r}_3, \vec{r}_1, \vec{r}_2) \) then \( \Pi(P) = 2 \) by first interchanging 3 and 1, and then 3 and 2. The canonical example is that

\[ \Psi_0(\vec{r}_1, \vec{r}_2) = -\Psi_0(\vec{r}_2, \vec{r}_1) \implies \int d\tau (\Psi_0(\vec{r}_1, \vec{r}_2) + \Psi_0(\vec{r}_2, \vec{r}_1)) = 0 \quad (2.24) \]

which, physically, states that the probability of having two fermions* in the same state, inte-

*of the same particle type, for instance proton or neutron
2.1. Many-Body Quantum Mechanics

grated over any region, is exactly zero. Equation (2.24) is indeed satisfied by the two-body Slater determinant

\[ \Psi_0(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) - \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)) \]

2.1.4 The Hartree-Fock Method

It is often the case that we will take a Slater determinant as an ansatz for a ground state, but there is no guarantee that a Slater determinant of single-particle ground state wave-functions, \( \phi_i(\vec{r}) \), will physically correspond to the collective ground state in the presence of particle interactions. The Hartree-Fock method is an application of the variational principle to this Slater determinant ansatz, \( |\Psi_0\rangle \), to make an optimal mean-field potential that minimizes any residual interactions between the single-particle states. To first order in perturbation theory, we know that the best approximation for the ground state energy of a Hamiltonian, \( \hat{H} \), is

\[ E_{\text{g.s.}} = \langle \Psi_0 | \hat{H} | \Psi_0 \rangle \]

Hence, the natural variational condition in this case is

\[ \delta \left( \frac{E_{\text{g.s.}}}{\langle \Psi_0 | \Psi_0 \rangle} \right) = 0 \] (2.25)

It was shown, by use of Lagrange multipliers, that Equation (2.25) gives the unconstrained problem known as the “Hartree-Fock equation”

\[ -\frac{\hbar^2}{2m_N} \nabla^2 \phi_a(\vec{r}) + V_{\text{HF}}(\{\phi_i(\vec{r})\})\phi_a(\vec{r}) = \varepsilon_a \phi_a(\vec{r}) \]

\[ i = 1, 2, \ldots, A \quad \text{and} \quad a = 1, 2, \ldots \] (2.26)

where we’ve assumed we’re working with \( A \) nucleons, and the Lagrange multipliers turned out to be the single-particle energies, \( \varepsilon_a \). This non-linear Schrödinger-type PDE can be solved iteratively with some guessed set of single-particle wave-functions [5].

In the case that we can set some Fermi surface, \( \varepsilon_F \), for our many-body state, Equation (2.26) can be rewritten in a simple way, in order to solve for the single-particle energies. That is, using a particle-hole occupation number representation (see Appendix C), Equation (C12) of Wick’s Theorem can be used to transform (2.26) into

\[ t_{ab} + \sum_{\varepsilon_c \leq \varepsilon_F} \sum_{\varepsilon_d} \nu_{c a b} = \varepsilon_a \delta_{a b} \] (2.27)

where the kinetic energy has be written with one-body matrix elements (OBMEs) in second quantization as in Equation (C13), and likewise for the anti-symmetrized version of the input interaction treated as a two-body operator as follows

\[ V = \frac{1}{2} \sum_{abcd} v_{abcd} \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_d \hat{c}_c \]
2.2. Nuclear Structure Theory

\[ \overline{v}_{abcd} \equiv v_{abcd} - v_{abdc} \]

Furthermore, once these single-particle energies are computed, a Hartree-Fock mean field can be constructed as

\[ \hat{H}_{HF} = \sum_a \varepsilon_a \hat{c}_a \hat{c}_a \]

giving the final Hartree-Fock ground state energy

\[ E_{HF} = \sum_{a \leq \varepsilon_F} t_{aa} + \frac{1}{2} \sum_{a,b \leq \varepsilon_F} v_{abab} \]

More details on how one can recast Equation (2.27) as an eigenvalue problem can be found in Section 4.6 of Suhonen [5]. Now that we have the mathematical tools to create a realistic many-body eigenspace, let’s apply them to nuclear structure.

2.2 Nuclear Structure Theory

The atomic nucleus represents the quintessential object to be handled by quantum many-body theory, since it is composed of protons and neutrons, which both obey quantum physics at this scale. Although the protons repeal each other by means of electric repulsion, the nucleus is held together by the strong nuclear force which binds both protons and neutrons collectively. Yet, this is not the only mechanism at play, since nucleons are spin-1/2 objects that obey the exclusion principle. This sets up a nuclear shell model, in analogy to the atomic shell model used to describe electron orbitals centred about the nucleus. Ultimately, nucleonic interactions and how those nucleons are physically structured together within the nucleus represents a fundamental problem in physics and natural philosophy; since without the stability of the nucleus, our reality would seize to exist.

2.2.1 The Basics

In the early 1930’s, Heisenberg noted that since the proton and neutron have such similar masses, currently reported as [18]

\[ m_p = 938.2720814 \text{ MeV} \]
\[ m_n = 939.5654134 \text{ MeV} \]

\[ \implies m_n - m_p \sim 2m_e \] 

then perhaps they could be considered as the same particle, only manifested as different quantum states. This particle was called the “nucleon,” and (remarkably) it can be described by the same group theoretic formalism as spin. The quantum number that flips a nucleon between its proton and neutron states is called “isospin,” and we’ll take the isospin convention that
\[ |p⟩ = |t = \frac{1}{2}, t_z = +\frac{1}{2}⟩, \quad |n⟩ = |t = \frac{1}{2}, t_z = -\frac{1}{2}⟩ \]

Of course, this is not an exact symmetry of quantum physics, since the proton and neutron masses are slightly different\(^*\) and the proton has a positive charge whereas the neutron is electrically neutral. However, since the Coulomb force is orders of magnitudes weaker than the strong force, it can be neglected, along with the small mass difference - thus making isospin formalism an important tool in basic nuclear physics.

A nucleus is composed of \( Z \) protons and \( N \) neutrons,\(^\dagger\) which are both composite objects made of up and down quarks. Thus, upon zooming in, a nucleus is (locally) like a quark-gluon soup with (global) structure. The mass number is defined as the number of nucleons

\[ A \equiv Z + N \]

and nuclei may be labelled as \((Z, A)\). Symbolically, atomic notation from chemistry is also used in nuclear physics, however it is simplified to

\[ ^AX# \rightarrow AX \]

since the chemical symbol, \( X \), is understood to label \( Z \), and the ionic charge, \( # \), is not often applicable. Alternatively, a nucleus may be referred to by its name appended with the mass number, for instance: Germanium-76 \( \overset{76}{\text{Ge}} \overset{32}{\text{(32, 76)}} \). We'll somewhat haphazardly switch between these notions. As usual, “isotopes” have the same proton number \( Z \), “isotones” have the same neutron number \( N \), and “isobars” have the same mass number \( A \). An interesting point about isobars is that, empirically, they are found to have the same nuclear radius

\[ R \approx r_0 A^{1/3}, \quad r_0 = 1.2 \text{ fm} \]  

(2.29)

Hence, the volume of a nucleus is proportional to \( A \).\(^\ddagger\) The mass of a nucleus, however, is a much more complicated beast.

**Semi-Empirical Mass Formula**

We can predict the mass of nucleus \((Z, A)\) via the formula

\[ m(Z, A) = Zm_p + (A - Z)m_n - BE(Z, A) \]  

(2.30)

where \( BE \) is the “binding energy.” The binding energy has a negative in Equation (2.30) since free nucleons which come together to make a stable nucleus will be sitting in an energy well via attractive forces, and this binding together will be contained as mass via relativity.\(^\S\) It is also experimentally relevant to report the “mass excess” of a nucleus, which is given by

---

*The proton is made of two valence up quarks and one valence down quark, whereas the neutron is made of one valence up quark and two valence down quarks. It turns out that the down quark’s constituent mass is heavier than the up’s, and the charge of the proton affects its mass via QED corrections.

\(^\dagger\)Typically \( Z < N \), since the positively charged protons repel each other electrostatically (long range force), but the neutrons hold the nucleus together via attractive strong interactions (short range force).

\(^\ddagger\)see the volume term of Equation (2.33)

\(^\S\)of course, here we have set \( c = 1 \)
\[ \Delta m \equiv m(Z, A) - A \cdot u \] (2.31)

where the “u” is the unified atomic mass unit (amu), defined as

\[ u \equiv 931.4940955 \text{ MeV} \] (2.32)

The binding energy is commonly modelled by the formula [16]

\[ BE(Z, A) = a_V A - a_S A^{2/3} - a_C \frac{Z(Z-1)}{A^{1/3}} - a_A \frac{(A-2Z)^2}{A} + \delta(Z, A) \] (2.33)

The first term of Equation (2.33) is the “volume term” \((V)\), which accounts for the strong interactions of nucleons with their neighbours under a femtometre range; the second is the “surface term” \((S)\), which corrects the first term for nucleons near the surface and introduces the liquid drop analog of surface tension; the third is the “Coulomb term” \((C)\), which gives electrostatic repulsions between protons; the fourth is the “asymmetry term” \((A)\), which models the Pauli exclusion principle for protons and neutrons and sets up their respective Fermi surfaces; and the fifth is the “pairing term” \((P)\), which accounts for pairwise spin coupling:

\[ \delta(Z, A) = \begin{cases} 0, & A = \text{odd} \\ +a_PA^{k_P}, & A = \text{even}, Z = \text{even} \\ -a_PA^{k_P}, & A = \text{even}, Z = \text{odd} \end{cases} \] (2.34)

Though the terms can all be theoretically justified, the parameters are fit empirically. For example, [25] lists them as

\[ a_V = 15.75 \text{ MeV}, \quad a_S = 17.8 \text{ MeV}, \quad a_C = 0.711 \text{ MeV} \]
\[ a_A = 23.7 \text{ MeV}, \quad a_P = 11.18 \text{ MeV}, \quad k_P = -1/2 \] (2.35)

When plotting for multiple isobars, the semi-empirical mass formula will give parabolic looking shapes, which are sometimes referred to as “mass parabolas.” An example of this can be seen in Figure 3.2, which depicts the double-beta decay of \(^{48}\text{Ca}\).

### 2.2.2 Nuclear Shell Model

The pioneers of nuclear structure theory noticed that nuclei would undergo discrete looking jumps in properties like energy levels around certain \(Z\) and \(N\). The numbers for which \(Z\) and \(N\) would display this phenomenon were called “magic numbers.” It was eventually realized that this pattern mimicked the electron orbital shell structure seen in atomic physics. Hence, it was proposed that both protons and neutrons occupy their own respective shells. This idea is somewhat puzzling in nuclear physics, since atomic orbitals are set up via quantization of the electron revolving around a centrally attractive object.* But, what are the protons and neutrons inside a nucleus orbiting - a mean field set up by their neighbours? Nonetheless, the nuclear shell model (ShM) has been successful in predicting nuclear properties [16].

*namely, the nucleus
2.2 Nuclear Structure Theory

Figure 2.1: Oxygen-16, as represented by the nuclear shell model. Both the protons (depicted by red balls) and the neutrons (depicted by blue balls) have been filled in their own respective shells. Here we’ve shown the ground state, which fills the single-particles in their orbits starting from \(0s_{1/2}\) to \(0p_{1/2}\), and portrays no excitations to higher orbits in the \(sd\)-shell or beyond. The spectroscopic notation used to label the orbits is explained in Figure 5.5 of [27], except we count the principle quantum number by shifting down by 1.

Nuclear shells are inherently related to the Pauli exclusion principle, since the nucleon is a fermion. What makes the ShM distinct from atomic orbitals, is that since the proton and neutron are different particle types (they have different isospin), they each have their own shells to fill, in tandem. For example, Figure 2.1 shows the ground state filling of \(^{16}\)O. To obtain the correct quantization of the shells, one begins with a QHO potential (see Section 2.1.1), which was found to be a good leading order approximation because it naturally describes self-bound systems [26]. The inclusion of spin-orbit coupling (that is, the addition of an \(\vec{S}\cdot\vec{L}\)-dependent term in the nuclear potential) will split the QHO shells and (magically) reproduce the observed magic numbers. A good visual description of reproducing the magic numbers is given in Figure 5.5 of Krane [27], which starts with a phenomenological Woods-Saxon potential\(^\ast\) and then adds in spin-orbit splitting. Overall, the ShM has acted as a paradigm for understanding the behaviour of nuclei [26], and thus it is a common first step in nuclear structure theory. Adding in nuclear interactions to capture dynamics within the shells, then, should give a good description of nuclear physics.

2.2.3 Nuclear Interactions

Ultimately, the strong nuclear force is an emergent phenomenon, which arises from the strong interaction between quarks, as governed by quantum chromodynamics (QCD). Quarks, as fermions, interact via the exchange of gluons, the boson which mediates the strong interaction. The QFT which describes this physics is referred to as QCD, since the “charge” of the strong interaction obeys SU(3) symmetry and is labelled by the three colours: red, green, and

\(^\ast\)this creates similar bound states to the QHO, but it is tailored to nuclear phenomenology
2.2. Nuclear Structure Theory

blue, and their corresponding anti-colours. Quarks will confine into colour neutral hadrons: either baryons (a bound set of three quarks)\(^*\) or mesons (a bound pair of a quark and anti-quark).\(^\dagger\) Stepping back in energy scale, one can view the strong interaction less precisely as an exchange of mesons\(^\ddagger\) between baryons, which is sometimes called “quantum hadrodynamics.” This emergence in nuclear physics can be seen schematically in Figure 2 of [28].

**Phenomenological**

The baseline theoretical tool to build nuclear interactions is, obviously, nuclear phenomenology [29, 30]. That is, one begins with mean-field\(^§\) or effective\(^¶\) field theory perturbative methods, and then designs a particular potential in order to reproduce nuclear properties like: binding energies, energy levels, and so on. Using a large body of experimental data for a chosen nucleus (or several), phenomenologists tune the interaction parameters to make their theoretical calculations fit with the measured values. This is often done beginning with a shell model approach, as was done for the GXPF1A interaction [31, 32], which is specifically designed to give good nuclear predictions for nuclei which have their predominate nucleon excitations within the \(pf\)-shell. Historically, this has been a successful approach - but it is not ab initio. The ultimate goal in nuclear physics is to build nuclear structure from a framework rooted in QCD; so phenomenological interactions are simply a means to an end.

**Chiral Effective Field Theory**

Another more fundamental approach to nuclear interactions is to use an effective field theory that reproduces low-energy QCD. A modern technique in this vain, which has proven to be successful for nuclear structure theory [7], is known as “chiral effective field theory” (\(\chi\)EFT). From a breakthrough paper by Weinberg [33], it was realized that chiral symmetry breaking in QCD Lagrangians can be used to build an EFT which reconstructs Yukawa’s original pion propagator theory [34] and higher-order corrections to nuclear forces [35]. In practice, techniques pioneered by [36, 37] can be used to perturbatively expand QCD in terms of a chosen energy cutoff scale, \(\Lambda\), to capture low-energy QCD.\(^∥\) The advantage with this formalism is that it gives theorists a way to distinguish between leading order (LO), next-to-leading order (NLO), next-to-nexto-to-leading order (N\(^2\)LO), \ldots contributions. This is typically done using a “power counting” scheme in \(\nu\)-powers of the expansion parameter, \((Q/\Lambda)^\nu\), which can be seen in Figure 2.2. Through this process, physics from neglected degrees of freedom is captured in short-range contact interactions which contain a number of “low-energy constants” (LECs) to

\(^*\)for example: a proton, neutron, or delta baryon
\(^\dagger\)for example: a pion, rho meson, or omega meson
\(^\ddagger\)mesons indeed are bosons, so they act as the force carrier of the strong nuclear force
\(^§\)treating a nucleon as affected by the potential of the collective interactions of its neighbouring nucleons
\(^¶\)treating mesons as the force carriers between baryons, built from a low-energy theory of QCD and hence taking the nucleus as a “soup” of quark-gluon structures
\(^∥\)note that the chiral symmetry breaking scale is at \(\Lambda \approx 1\) GeV (the nucleon mass)
2.2. Nuclear Structure Theory

Figure 2.2: “Hierarchy of nuclear forces in $[\chi\text{EFT}]$” taken from Figure 1 of [7]. Nucleons and pions are depicted as solid and dashed lines respectively in the perturbative nuclear Feynman diagrams. The dots represent vertex type, see [7] for more details.

be calculated perturbatively or fit to data (like nucleon-nucleon phase shifts), such as with the so-called EM 1.8/2.0 interaction [38]. Once these Hamiltonians have been constructed, one can use them as input for a nuclear many-body method to model nuclear structure.

2.2.4 Nuclear Many-Body Methods

We’ve already introduced one of the staple many-body methods, the nuclear ShM (see Section 2.2.2 above). But today, there exist plenty of competing nuclear many-body methods on the market (IM-SRG, CC, NR-EDF, QRPA, IBM, etc) [13], each with their own advantages and drawbacks. A glaring irony of these quantum many-body techniques is that they cannot go beyond the nucleon-nucleon (2N) level, since higher body effects like three-nucleon (3N) configurations are still too mathematically complex. One method which remedies this issue is the in-medium similarity renormalization group (see Chapter 5). By redefining normal ordering with respect to the nuclear medium (see Section 5.3), this method can capture the bulk effects of 3N physics using 2N technology! This will surely make appreciable differences in nuclear structure calculations, such as those for double-beta decay.
2.3 Beta Decay

Before we move on to double-beta decay, let’s first introduce one of its defining components: single-beta decay. There are two main types of beta decay - in which either the neutron decays into a proton and emits an electron (to conserve charge) with a electron anti-neutrino (to conserve lepton number), or the proton decays into a neutron, positron, and electron neutrino.

\[ n \rightarrow p + e^- + \bar{\nu}_e \quad \text{or} \quad p \rightarrow n + e^+ + \nu_e \]

The former is often called \( \beta^- \) decay, whereas the latter is \( \beta^+ \) decay. By experimental convention, we’ll focus on the former, and simply call this “beta decay”: \( \beta^- \rightarrow \beta^+ \). An interesting note is that \( \beta^+ \) cannot happen spontaneously in free space, since the final state has more rest mass (see Equation (2.28), and note that \( m_{\nu} \approx 0 \)). However, the proton can decay within a nucleus, because it can be excited (thus deriving energy/mass) through strong interactions with neighbouring nucleons. Both \( \beta^- \) and \( \beta^+ \) nuclear beta decay led to the discovery of the neutrino, as posited by Pauli in 1930 to solve the problem of missing energy in laboratory measurements of beta-radioactivity [39]. At this point, early particle physicists were confident that they were on their way to completing a theory of fundamental physics, but even a decay as simple as beta decay kept more secrets lurking within.

2.3.1 Parity Violation

Parity is a spacial coordinate transformation whereby one axis is flipped. By classical intuition, such a simple inversion wouldn’t seem to change the laws of physics, so parity could be assumed to be a symmetry of the universe. Indeed, parity is conserved for electromagnetic and strong processes, but in 1956 it was realized by Lee and Yang that not enough evidence existed to establish or refute parity conservation in the weak sector [40]. Subsequently, parity violation was found in the beta decay of \( ^{60}\text{Co} \) [41], and a full \( V-A \) theory of the weak interaction was rapidly developed [42, 43]. For the Standard Model, parity happens to be maximally violated in that: only left-handed particles and right-handed anti-particles participate in the weak interaction. A pedagogical introduction to the particle physics behind \( V-A \) theory can be found in [44].

The constants which describe parity violation are the vector coupling constant, \( g_V \), and the axial-vector coupling constant, \( g_A \). Modern experiments are still being designed to improve the measurement of the \( V-A \) constants, such as [45]. Accordingly, we’ll take the values as

\[ g_V = 1 \quad \text{and} \quad g_A = 1.27 \]

These constants will come up frequently in the equations describing beta decay.
2.3. Beta Decay

2.3.2 Allowed Fermi Transition

Among many forbidden and super-allowed beta transitions [5], there are two main leading-order* modes to beta decay: the Fermi (F) transition [46], and the Gamow-Teller (GT) transition [47]. For the Fermi case, the spins of the electron and the neutrino are anti-aligned, hence they couple to spin $S = 0$. Hence, the total spin of the nuclear state remains unchanged, giving the selection rule $\Delta J = 0$. Such a simple selection rule is clearly modelled by using the identity operator taken as a spherical tensor

$$\hat{O}_F \equiv g_V \mathbb{1} \tau^+$$ (2.36)

along with the isospin operator, $\tau^+$, which will flip the state of the nucleon from neutron $t_z = -1/2$ to proton $t_z = +1/2$ in accordance with the beta decay. To find the reduced OBMEs for the Fermi transition (to be used in Equation (C26) for a nuclear matrix element calculation), we’ll omit the isospin operator† and apply Equation (B11) to (2.36), giving

$$\langle a || \hat{O}_F || b \rangle \propto \delta_{n_a n_b} \delta_{l_a l_b} \delta_{j_a j_b} \hat{u}$$

This scenario is remarkably more simple than the Gamow-Teller case (see below), and more so compared to neutrinoless double-beta decay two-body matrix elements (TBMEs), which are tediously derived in Chapter 4.

2.3.3 Allowed Gamow-Teller Transition

The Gamow-Teller mode is characterized by the spin alignment of the emitted particles in the beta decay. Therefore they couple to spin $S = 1$, yielding the selection rule $\Delta J = 0, \pm 1$. This change in angular momenta can be modelled by the use of a Pauli operator as follows

$$\hat{O}_{GT} \equiv g_A \hat{\sigma} \tau^+$$ (2.37)

To obtain the reduced matrix elements of the Gamow-Teller operator, $\langle l \frac{1}{2}; j || \hat{O}_{GT} || l' \frac{1}{2}; j' \rangle$, we’ll omit the analysis of the isospin operator,† and instead start by looking at the matrix elements of the spin operator (with $\hbar \neq 1$)

$$\hat{S} = \frac{1}{2} \hbar \hat{\sigma}$$ (2.38)

We’ll take our quantization axis as the $z$-axis, and update the $z$-component of the spin operator to a vector (rank $L = 1$) spherical tensor, $\hat{S}_z \rightarrow \hat{S}_1$. The non-reduced matrix elements of $z$-component of Equation (2.38) are built by acting on spin-1/2 states

$$\langle \frac{1}{2} m || \hat{S}_1 || \frac{1}{2} m' \rangle = m' \hbar \delta_{mm'}$$ such that, $m, m' = \pm \frac{1}{2}$ (2.39)

To reduced these matrix elements, we can simply use the Wigner-Eckart Theorem of Equation (B9), labelling the projected spherical tensor rank as $M$, giving

---

*as taken in the non-relativistic limit of the weak interaction
†since this will introduce a Kronecker-delta of some form, depending on the chosen isospin formalism
2.3. Beta Decay

\[ \langle \frac{1}{2} m' | \vec{S}_M | \frac{1}{2} m \rangle = (-1)^{\frac{1}{2} - m'} \left( \frac{1}{2} - m' \ M \ \frac{1}{2} - m' \right) \langle \frac{1}{2} | \vec{S} | \frac{1}{2} \rangle \]  

(2.40)

Plugging Equation (2.39) into Equation (2.40) will yield $0 = 0$ unless $m' = m$ on the LHS, and $-m' + M + m = 0$ on the RHS by Equation (A24), $\implies M = 0$. It can be easily found that

\[ \langle \frac{1}{2} | \vec{S} \rangle \rangle = \left( \frac{-1}{2} \ 1 \ \frac{1}{2} \ 
\begin{pmatrix} 1 \\
0 \\
\frac{1}{2}
\end{pmatrix}
\right) = \frac{1}{\sqrt{6}}
\]

so, overall, we obtain

\[ m' h = \frac{(-1)^{\frac{1}{2} - m'}}{\sqrt{6}} \langle \frac{1}{2} | \vec{S} | \frac{1}{2} \rangle \implies \langle \frac{1}{2} | \vec{S} | \frac{1}{2} \rangle = \frac{\sqrt{6}}{2} h = \sqrt{\frac{3}{2}} \]

(2.41)

where we’ve dropped the “rank 1” subscript for the $\vec{S}$; which is to be understood as the spherical tensor operator* of the $z$-component of the spin operator, as opposed to the (bolded) vector spin operator. However, since the projected spin quantum number should be $\pm \frac{1}{2}$ on any axis, Equation (2.41) will hold for any component of the spin treated as a vector spherical tensor, and so we could† explicitly write

\[ \langle \frac{1}{2} | | \vec{S}_z, \vec{S}_y, \vec{S}_x | \frac{1}{2} \rangle = \frac{3}{2} h \]

(2.42)

Finally, putting Equation (2.38) and (2.41) together gives us

\[ \langle \frac{1}{2} | | \vec{S} | \frac{1}{2} \rangle = \frac{\sqrt{6}}{2} h = \sqrt{\frac{3}{2}} h \]

(2.42)

Now we consider a spin-1/2 particle with total angular momentum, $j$, via the $ls$-coupling $\Delta(l \frac{1}{2} : j)$. Since the Pauli operator is a vector spherical tensor operator, like the spin operator, we may apply Corollary B.2.4 to it in this $ls$-coupling. Using Equation (B27) gives

\[ \langle l s : j | | \vec{\sigma} | l' s' : j' \rangle = -\delta_{ll'} \delta_{ss'} (-1)^{l+2j+j' + 1} \langle \frac{1}{2} | | \vec{\sigma} | \frac{1}{2} \rangle \]

(2.43)

and plugging Equation (2.42) into (2.43) yields the reduced matrix elements

\[ \langle l \frac{1}{2} : j | | \vec{\sigma} | l' \frac{1}{2} : j' \rangle = \sqrt{6} \delta_{ll'} \delta_{jj'} (-1)^{l+j+\frac{3}{2}} \langle \frac{1}{2} | | \vec{\sigma} | \frac{1}{2} \rangle \]

(2.44)

Thus, all that one needs to do to calculate the one-body reduced matrix elements of the Gamow-Teller operator of Equation (2.37) is compute (2.44), account for the isospin formalism, and multiply by the axial-vector coupling constant, $g_A$. Note that we need not anti-symmetrize Equation (2.44), since it doesn’t make physical sense to anti-symmetrize a one-body state. However, if we mathematically applied Equation (B31) and anti-symmetrized between $l$ and $s$, we would nonetheless find that

* hence it is bolded
† although we never will
\[ \langle l \frac{1}{2}; j | \hat{\sigma}|| l' \frac{1}{2}; j' \rangle = \langle l \frac{1}{2}; j | \hat{\sigma}|| l' \frac{1}{2}; j' \rangle \]
since \( l \) cannot take on half-integer values.

### 2.3.4 Quenching in Single-Beta Decay

It’s long been known, to the dismay of many theorists, that the predictions from Equation \( (2.44) \) in fact do not reproduce the experimental observations of single-beta decay [48]. To correct for these discrepancies, the axial-vector coupling constant is often set to one, \( g_A \rightarrow 1 \), or a “quenching factor” is multiplied by the GT operator. That is,

\[ q_f \sim \frac{1}{g_A} \approx \frac{1}{1.3} \approx 77\% \quad (2.45) \]

is multiplied by Equation \( (2.37) \). However, many different quenching factors (ranging from 0.6 to 0.9) have been proposed [13, 49], and they seem to be nucleus dependent! This inconsistency in the quenching factor begs a precarious question: where does quenching come from? Is it the axial-vector coupling constant in Equation \( (2.37) \) that is effectively quenched, or does \( q_f \) come from the “bare” GT matrix elements in \( (2.44) \) themselves, or a mixture of both?

In the case that it is all coming from the nuclear matrix elements, this implies that the chosen nuclear structure model may be able to account for quenching. In other words, perhaps not enough physics is being captured by the nuclear structure calculations of beta decay. For instance, those who work on the interacting ShM have stated that, given they could implement a full model space, then the problem of quenching will be solved within their framework [50, 51].

Thus, quenching may simply be a byproduct of having a “truncated basis space” (see Section 5.1). A somewhat related claim is that quenching indeed originates from the bare GT operator, due to an ill-considered analysis of the nuclear spectroscopic data [26]. However, all these proposals are still argued to this day, and many alternative explanations exist [13]. One of the largest effects, which may solve the problem of quenching, comes from the inclusion of meson exchange currents [52]. Overall, this important question has not been settled, and the debate is still very alive, in particular within the double-beta decay community [53]. For more on this phenomenon, see Section 3.1.4.

---

*These citations are for the case of double-beta decay, but quenching is assumed to be a shared problem between both single and double-beta decay (see Section 3.1.4).*
Chapter 3

Double-Beta Decay

The first theoretical suggestion of double-beta decay was made by Maria Goeppert-Mayer in 1935 [54]. For her contributions to nuclear physics, she won the Nobel prize in 1963 along with Wigner and Jensen, making her the second (and latest) female to win the prize, following Marie Skłodowska Curie. As discussed in Section 3.1.1 below, double-beta decay with the emission of two neutrinos (2νββ) was subsequently measured. Furthermore, since the self-conjugate nature of the neutrino has not been experimentally established, it has been suggested that the emitted neutrinos in 2νββ could annihilate [55, 56], leading to a lepton-number violating process known as “neutrinoless double-beta decay” (0νββ), covered in Section 3.3. The fundamental mechanisms behind 0νββ are theoretically unclear, as pointed out in Section 3.2.

3.1 Two-Neutrino Double-Beta Decay

The dominate mode of double-beta decay happens via the emission of two electron anti-neutrinos, as opposed to the neutrinoless case. A common schematic used to visualize this decay is a Feynman diagram, as seen in Figure 3.1 below. On the LHS of the diagram, we begin with two neutrons; and hence a charge of zero and a lepton number of zero. On the RHS of the diagram, we end with two protons, two electrons, and two electron anti-neutrinos; and hence a net charge of zero and a net lepton number of zero. The two electrons carry a charge of −2 and a lepton number of +2, and so they act to cancel the charge of the two protons; whereas the two electron anti-neutrinos carry a lepton number of −2 to cancel out the “electron-ness” of the final state. Thus, all the Standard Model quantum numbers are conserved in 2νββ.

Figure 3.1 is misleading since it makes double-beta decay appear as though it is simply two single-beta decays happening concurrently. However, this is not the case, since it is not possible for any arbitrary nucleus to undergo 2νββ sporadically. This is because the pairing term in the semi-empirical mass formula of Equation (2.33) yields an asymmetry in nuclei. For instance, considering isobars of mass A = 48, we see in Figure 3.2 below that it is energetically favourable for Potassium-48 to beta decay into Calcium-48, but it is not energetically favourable for Calcium-48 to beta decay into Scandium-48. It is, however, energetically favourable for Calcium-48 to double-beta decay into Titanium-48. Hence, we should keep in mind that

\[ \beta\beta \neq \beta + \beta \]

and that only nuclei lying close to the bottom of the mass parabolas, in the same kind of configuration as in Figure 3.2, represent double-beta decay candidates. This configuration is
3.1. Two-Neutrino Double-Beta Decay

Figure 3.1: The nuclear Feynman diagram for double-beta decay. In terms of a nucleus, the decay is read as: \((Z, A) \rightarrow (Z + 2, A) + 2e^- + 2\bar{\nu}_e\)

favoured experimentally since one can be confident that starting with a sample of \((Z, A)\) and yielding products of \((Z + 2, A)\) has not occurred simply by two beta decays in a row.

3.1.1 Experimental Confirmation of \(2\nu\beta\beta\)

A list of important historical events involving double-beta decay can be seen in Table 4 of [58]. The two-neutrino double-beta decay was theorized half a century before it was first directly measured in the laboratory, for the nucleus \(^{82}\text{Se}\) [59]. In fact, even indirect evidence for \(2\nu\beta\beta\) by means of geochemical analysis involving \(^{130}\text{Te}\) took 15 years following Goeppert-Mayer’s proposal [60]. Such experimental confirmations have, in turn, proven useful for theoretical studies of nuclear structure [61]. This is since one can benchmark nuclear many-body predictions of a rare decay against actual experimental data, and give insight into mysteries surrounding this decay, like quenching for instance (see Section 3.1.4 below).

Since the first measurement of double-beta decay in \(^{82}\text{Se}\), many more direct decays have been observed in numerous nuclei, such as: \(^{48}\text{Ca}\), \(^{76}\text{Ge}\), \(^{96}\text{Zr}\), \(^{100}\text{Mo}\), \(^{116}\text{Cd}\), \(^{130}\text{Te}\), \(^{136}\text{Xe}\), and \(^{150}\text{Nd}\). These nuclei are even-even, of course, and have similar mass parabolic arrangements to those in Figure 3.2. Measurements of \(2\nu\beta\beta\) are still on-going, and experimental techniques in this field are continually improving. A leading experiment in this search is known as NEMO-3. For instance, at the time of writing, the most recent measurement of double-beta decay in \(^{48}\text{Ca}\) is given by the NEMO-3 Collaboration [62], which quotes the half-life as

\[
T_{1/2}^{2\nu}(^{48}\text{Ca}) = [6.4^{+0.7}_{-0.6}(\text{stat})^{+1.2}_{-0.9}(\text{syst})] \times 10^{19} \text{yr}
\]  

(3.1)

Other half-lives have been compiled in [63].
3.1. Two-Neutrino Double-Beta Decay

Figure 3.2: Even (orange) and odd (green) mass parabolas of $A = 48$ isobars, showing the double-beta decay of $^{48}\text{Ca}$ into $^{48}\text{Ti}$. To calculate the parabolas, we used Equations (2.30), (2.31), and (2.33), where we took the parameters from (2.35), but refit $a_C$ and $a_A$ to reproduce the precise mass excess of $^{48}\text{Ca}$ and $^{48}\text{Sc}$ given by [57]. The blue arrows represent $\beta^-$ decay, the purple arrows represent $\beta^+$ decay, and the red arrow is the double-beta decay. Notice that $^{48}\text{Ar}$ could, hypothetically, double-beta decay into $^{48}\text{Ca}$, but this would be difficult to distinguish from two beta decays in a row, following the blue arrows. Also note that $^{48}\text{Ca}$ could beta decay into $^{48}\text{Sc}$, because of its minutely lower mass, but this is highly repressed relative to double-beta decay. This is not the case for many double-beta decay candidates, for example in Figure 1 of [53], where clearly $\Delta m(^{76}\text{Ge}) < \Delta m(^{76}\text{As})$, in contrast to $\Delta m(^{48}\text{Ca}) \approx \Delta m(^{48}\text{Sc})$.

3.1.2 $2\nu\beta\beta$ Half-Life Formula

As presented by Tomoda [64] in their Equation (3.26), based on work by Doi et al. [65, 66], the $2\nu\beta\beta$ half-life formula can be written as

$$[T_{1/2}^{2\nu}]^{-1} \approx G^{2\nu}|M^{2\nu}|^2$$  \hspace{1cm} (3.2)

where $G^{2\nu}$ is known as the “phase (space) factor,” which incorporates the interface between particle and nuclear physics, and will be discussed more below; $M^{2\nu}$ is the “nuclear matrix element” (NME), which incorporates nuclear structure theory; and Equation (3.3) indeed obeys (F11). The “approximately equals” sign mainly comes from neglecting the lepton energies relative to the nuclear excitation energies, which are strategically replaced by averages [64]. From now on, such approximation signs will be dropped, as they are understood in this context.

As made explicit in [67], it has become customary to rewrite Equation (3.2) as
3.1. Two-Neutrino Double-Beta Decay

\[ [T_{1/2}^{2\nu}]^{-1} = G^{2\nu} g_A^4 |M^{2\nu}|^2 m_e^2 \]  

(3.3)

where \( g_A \) is the axial-vector coupling constant from Section 2.3.1, and the units of \( m_e \) are taken as MeV. This is convenient since it puts the units of the phase factor into inverse years, and any hypothetical renormalization of \( g_A \) can be handled a posteriori. However, it may become cumbersome when looking for values of the phase factor in the literature, since the labelling for \( G^{2\nu} \) is not clearly distinguished between Equation (3.2) and (3.3).

\( 2\nu\beta\beta \) Phase Factor

From the time leading up to its publication, [64] had reformulated the theory of double-beta decay into the construct still used to this day. They also presented numerical results for the phase factor, which they called the “lepton phase-space integral,” given in their Equation (3.28). However, a more modern and sophisticated analysis has been done in [67] and [68], which we will refer to for our numerical values of \( G^{2\nu} \). Ultimately, the calculation of these values involves how the relativistic electron wave-functions of double-beta decay interact with the Coulomb potential, whilst taking screening effects and a realistic finite nuclear size into consideration.

Additional nuclear physics is also ingrained into \( G^{2\nu} \), but by a remarkable coincidence* this dependence cancels out - thus leading to the succinct separation of the phase factor and the NME seen in Equation (3.3) above. We will not go into the details of this physics whatsoever, and instead leave it to the expert analysis as presented in [64, 67–69]. For instance, [67] (printed below) and [63, 68, 69] all give similar values for \( 2\nu\beta\beta \) in \(^{48}\text{Ca} \), among others

\[ G^{2\nu}(^{48}\text{Ca}) = 1.555 \times 10^{-17} \text{yr}^{-1} \]  

(3.4)

Example 3.1

Let’s make a reverse prediction of the NME for the double-beta decay of \(^{48}\text{Ca} \) into \(^{48}\text{Ti} \). That is, taking the theoretical value in Equation (3.4) above and the experimental value in Equation (3.1), treating the latter as having indefinite precision, setting \( g_A = 1.27 \) and \( m_e = 0.511 \text{MeV} \), and plugging all these values into Equation (3.3), we should expect to see an NME in the range of

\[ M^{2\nu} \approx 0.03846 \text{MeV}^{-1} \]  

(3.5)

However, considering the current status in nuclear structure theory, producing this number from scratch will not necessarily happen. The reason for the discrepancies seen will be commented on in Section 3.1.4 below, but first let’s outline how these matrix elements are calculated.

*as first noted by [64] and explicitly shown in [67]
3.1.3 $M^{2\nu}$ Matrix Elements

As with single-beta decay, the modes of $2\nu\beta\beta$ are the Fermi (see Section 2.3.2) and Gamow-Teller transitions (see Section 2.3.3). Thus, the NME from Equation (3.3) can be split up as

$$M^{2\nu} = M^{2\nu}_{GT} - \left( \frac{g_V}{g_A} \right)^2 M^{2\nu}_F$$

(3.6)

where $g_V$ and $g_A$ are the vector and axial-vector coupling constants respectively, as introduced in Section 2.3.1. However, as shown in Section 7.1 of [66], we can make the simplification that

$$|M^{2\nu}_{GT}| \gg |M^{2\nu}_F|$$

since “nearly all the Fermi strength goes into the isobar analog state in the daughter, so that $M^{2\nu}_F$ can be neglected.” [70] pp. 488

From the derivation of Equation (3.3), it can be shown that the dominant GT component for a $2\nu\beta\beta$ decay from the $0^+$ ground state of a parent nucleus to the $J^+$ state of the daughter nucleus is given by [48, 64, 67, 69, 71]

$$M^{2\nu} \approx M^{2\nu}_{GT} = \frac{1}{\sqrt{J+1}} \sum_k \langle J^+_f \mid \hat{\sigma}_+ | 1^+_k \rangle \langle 1^+_k | \hat{\sigma}_+ | 0^+_i \rangle [E_k + E_d(J)]^{J+1}$$

(3.7)

where $i$ represents the initial state, of the parent nucleus; $k$ represents the intermediate state, of the virtual intermediate odd-odd nucleus; and $f$ represents the final state, of the daughter nucleus. The NMEs for the individual GT operators in the numerator of Equation (3.7) are evaluated simply by using (2.44) within one’s chosen nuclear structure model. $E_k$ are the excitation energies of the intermediate state, as measured relative to the intermediate nucleus' ground state. $E_d(J)$ is simply an energy displacement defined by

$$E_d(J) \equiv \frac{1}{2} Q_{\beta\beta}(J^+) + \Delta M$$

and, $\Delta M \equiv M_k - M_i$

(3.8)

where $Q_{\beta\beta}$ is the $Q$-value of the double-beta decay, and $M_k, M_i$ are the masses of the intermediate and parent nuclei respectively. As usual, the $Q$-value is defined as the sum of the masses of the initial configuration minus the sum of the masses of the final products

$$Q_{\beta\beta} = M_i - M_f - 2m_e$$

(3.9)

where here we’ve neglected the mass of the two neutrinos, $m_{\nu_e} \approx 0$, and of course $m_e$ is the mass of the electron ejected from the corresponding beta decay.

A common ambiguity within the literature [48, 71] is how all these energies and masses are defined. For instance, we assume that the parent nucleus is atomically neutral - that is, it has $Z$ atomic electrons in its electron cloud. The daughter nucleus will therefore also have $Z$ atomic electrons, but it has $Z+2$ protons since two of the parent neutrons have simultaneously beta decayed. Thus, the daughter nucleus is actually atomically charged by +2 units of $|e|$, and the $M_f$ in Equation (3.9) above should actually be labelled as $M_f^{2+}$ instead. Since this is cumbersome, no one writes this; so to make the distinction clear, let’s at least use a superscript $a$ to denote when masses are atomically neutral. That is, we may rewrite Equation (3.9) as
3.1 Two-Neutrino Double-Beta Decay

\[ Q_{\beta\beta} = M_i^a - (M_f + 2m_e) = M_i^a - M_f^a \]  \hfill (3.10)

Plugging Equation (3.10) into (3.8) and setting \( J_f^+ = 0^+_f \) gives us

\[ E_d(0) = \frac{1}{2} (M_i^a - M_f^a) + M_k - M_i^a = M_k^a - m_e - \frac{1}{2} (M_i^a + M_f^a) \]  \hfill (3.11)

where we note that we’ve used \( M_k = M_k^a - m_e \), since the virtual intermediate nucleus would have \( Z \) atomic electrons and \( Z + 1 \) protons, and hence \( M_k \) is atomically charged by \(+1\) units of \(|e|\). We can’t take that electron mass from the beta decay, since they’ve already been absorbed by the \( Q \)-value via Equation (3.10). Putting Equation (3.11) into (3.7) with \( J_f^+ = 0^+_f \) yields

\[ M^{2\nu}(0^+ \to 0^+) = \sum_k \left[ \langle 0^+_f | \bar{\sigma} \tau^+ | 1^+_k \rangle \langle 1^+_k | \bar{\sigma} \tau^+ | 0^+_i \rangle \right] \frac{E_k - E_{g.s.}^k}{M_k - m_e - \frac{1}{2} (M_i^a + M_f^a)} \]  \hfill (3.12)

where we’ve redefined the excitation energies to make it computationally explicit that they are relative to the intermediate nucleus’ ground state, which is valid as long as \( E_k^g \) and \( E_{g.s.}^k \) are measured relative to the same scale. Also, notice that (although they are labelled by \( k \)) both \( E_k^g \) and \( M_k \) don’t actually change in value over the summation; only \( E_k^g \) and \( 1^+_k \) do.

An important note is that the closure approximation (see Section C.3.1) is insufficient for two-neutrino double-beta decay [72]. This leads to an immediate problem, since obtaining a complete set of intermediate states is not generally possible. This will induce discrepancies in predicting values for equations like (3.7) and (3.12), since a truncation will have to be made in the amount of states used in the summation. More on this will be discussed in Section 7.1.

Finally, one may ask, “what are the dominate final state contributions to the \( 2\nu\beta\beta \) decay in general, using Equation (3.7)?” This kind of analysis has been conducted in [71] and [73] for \( ^{48}\text{Ca} \) where they find that the decay \( 0^+ \to 2^+ \) gives negligible contributions to the half-life. Hence, higher lying final states will be neglected, and most authors will focus on \( 0^+ \to 0^+ \) first, since it generally dominates for double-beta decay.

Example 3.2

We’ll now set up the \( M^{2\nu} \) matrix elements for the case of \( ^{48}\text{Ca} \) double-beta decaying into \( ^{48}\text{Ti} \) via the \( 0^+ \to 0^+ \) mode. The virtual intermediate nucleus will be \( ^{48}\text{Sc} \), which has a \( 6^+ \) ground state [74, 75]. To obtain the atomic masses required in the denominator of Equation (3.12), we’ll take precision values from [76] for \( ^{48}\text{Ca} \), [18] for the electron mass, and [77] otherwise. In Equation (3.11) we obtain

\[ m_e = 0.5109989461 \text{ MeV} \]
\[ u = 931.4940955 \text{ MeV} \]
\[ M_i^a = M(^{48}\text{Ca}) = 47.95252276 \text{ u} \]
\[ M_k^a = M(^{48}\text{Sc}) = 47.952231 \text{ u} \]
3.2 From Two Neutrinos to None

\[ M_f^2 \doteq M^{(48}\text{Ti}) = 47.9479463 \text{ u} \]
\[ \implies M_k^a - m_e - \frac{1}{2}(M_t^a + M_f^a) = 1.348701071 \text{ MeV} \]  

(3.13)

Notice that had we used Equation (3.8) with a precision measurement of the \( Q \)-value, like \( Q_{\beta\beta} = 4.26798 \text{ MeV} \) from [78], then we would have arrived to roughly the same \( E_d \) as above.

Putting Equation (3.13) into Equation (3.12) gives us

\[ M^{2\nu}(^{48}\text{Ca}^{0+} \rightarrow ^{48}\text{Ti}^{0+}) = \sum_k \frac{\langle ^{48}\text{Ti}^{0+} || \hat{\sigma}\tau^+ || ^{48}\text{Sc}^{1+}_k \rangle \langle ^{48}\text{Sc}^{1+}_k || \hat{\sigma}\tau^+ || ^{48}\text{Ca}^{0+} \rangle}{E'_k - E(^{48}\text{Sc}^{6}_{g.s}) + 1.348701071 \text{ [MeV]}} \]  

(3.14)

where the superscripts on the nuclei represent \( J^+ \), i.e., total angular momentum and parity, as opposed to atomic charge (as used in chemistry notation).

### 3.1.4 Quenching in \( 2\nu\beta\beta \)

Given the GT operator of single-beta decay requires quenching (see Section 2.3.4), then it is reasonable to presume that \( M^{2\nu} \) in Equation (3.7) is also quenched. Since the \( M^{2\nu} \) matrix elements are composed of two copies of the GT operator, all that is done to “quench” double-beta decay is multiply the matrix elements by \( q^2_f \), as in Equation (2.45). Upon squaring the NME, the quenching will roughly cancel the four copies of \( g_A \) in Equation (3.3). Thus, what many researchers do is model single-beta decay quenching factors within their nuclear structure model, and then use these \( q_f \) for double-beta decay [26], and make half-life predictions via

\[ M^{2\nu} \rightarrow q^2_f \cdot M^{2\nu} \]

Though this procedure seems simple enough, it is important to point out, once again, that the community is still at odds with how to interpret the phenomenon of quenching in the context of double-beta decay [13]. In fact, the range in appropriate quenching factors for beta decay suggests that it’s the GT NMEs which are the source of quenching, as opposed to a renormalization of \( g_A \) [49]. Therefore, in this research, we will only present unquenched results.

### 3.2 From Two Neutrinos to None

Neutrinoless double-beta decay was first proposed by Wendell H. Furry [55], based on the realization that a neutrino could be self-conjugate and the physics of single-beta decay would remain unchanged. Hence, the neutrino in \( 2\nu\beta\beta \) could annihilate, leaving only two protons and two beta particles in the final state, as in Figure 3.3. This process could also happen via the emission of a neutrino at the top weak vertex and an absorption at the bottom, and visa versa. Looking at Figure 3.3, it does not take long to realize that something with \( 0\nu\beta\beta \) is not quite kosher within the framework of the Standard Model. To highlight these discrepancies, we’ll explore the following questions:
Would $0\nu\beta\beta$ confirm that: Lepton number is violated?

By definition, neutrinoless double-beta decay begins with two neutrons, and ends with two protons and two electrons. We can see that charge is conserved, however the net change in electron lepton number of Figure 3.3 is non-zero:

$$\Delta L^{0\nu} = L_f - L_i = 2 - 0 = 2 \neq 0$$

This is a significantly disturbing feature of $0\nu\beta\beta$: it requires lepton number violation (LNV). Such a violation has never been measured before, and lepton number has been held as a fundamental conserved quantity in the Standard Model. With this said, many studies [79–82] and searches [83–85] for lepton number violation have already been conducted.

A discovery of LNV would entail that the Standard Model of particle physics is fundamentally incomplete, since much of it is built upon symmetries and the the conservation of their corresponding quantum numbers. In the case of experimentally confirmed LNV, physicists would need to develop new theories Beyond the Standard Model (BSM). An exceptionally exciting aspect of LNV is that it can* account for baryogensis in such a way that explains the matter/anti-matter asymmetry in the universe [86, 87]. Thus, if found, $0\nu\beta\beta$ would have profound cosmological implications, since it can be thought of as a lepton generating decay.

* [86] shows specifically that this is possible without the need for grand unification.

In conclusion, the answer to the title of this sub-section is: true.
3.2. From Two Neutrinos to None

Would $0\nu\beta\beta$ confirm that: The neutrino is its own anti-particle?

From Figure 3.1, it is clear that the only way that the emitted electron anti-neutrinos can annihilate is if the neutrino is its own anti-particle. Similarly, for the neutrino to be emitted from the top weak vertex (for instance) of Figure 3.3, and then absorbed at the bottom vertex, it must be able to flip chirality. That is, since the neutrino would be emitted from the top single-beta decay as a left-handed particle, to conserve chirality it must be right-handed to be absorbed in the bottom single-beta decay. As discussed further in the next question below, the only way this flip in chirality is possible is if the neutrino is its own anti-particle.

However, we know from the question above that we must admit $0\nu\beta\beta$ is a LNV process. Once a single LNV operator is incorporated into the Lagrangian, this induces many other potential LNV mechanisms, as described in detail by [13]. Most of these BSM mechanisms involve the exchange of a heavy particle, for instance a meson exchange current (MEC) as in Figure 3.4 seen below. Since a MEC involves the exchange a heavy\* particle, the nucleons involved in Figure 3.4 must be “closer” (on average) than those in Figure 3.3, and hence any MEC contribution is suppressed relative to the traditional $0\nu\beta\beta$. This dominance of the neutrino exchange diagram can be shown definitively within the framework of $\chi$EFT (briefly introduced in Section 2.2.3).

$\mapsto$ In conclusion, the answer to the title of this sub-section is: true.

Does $0\nu\beta\beta$ require that: The neutrino has a non-zero mass?

Mohapatra’s chapter in Current Aspects of Neutrino Physics gives an insightful overview into the theory (or lack thereof) behind the neutrino mass [88]. He points out that the initial $V-A$ model was developed in order to account for the parity violation\† in the neutrino for single-beta decay. This was built on the $\gamma^5$-invariance of the weak Lagrangian for all fermions, which was historically motivated by the presumed masslessness of the neutrino. In conjunction with $B-L$ being an exact symmetry, this initial parity violating theory yielded a precisely massless neutrino in the Standard Model (to all perturbative orders).

Ironically, further investigation into neutrino physics has established that this symmetry in the Standard Model must be broken. As the Cabibbo-Kobayashi-Maskawa (CKM) matrix dictates the ability for quark flavour to change via the weak interaction, the Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix predicted an oscillation of neutrino flavour [89, 90]. However, in order for the three mass eigenstates ($m_1, m_2, m_3$) of the neutrino to mix between its flavour eigenstates ($e, \mu, \tau$) during propagation, the neutrino must have a non-zero mass so that it can experience time in its rest frame.\‡ In 2015, Canadian scientist Arthur B. McDonald and Takaaki Kajita of Japan accepted the Nobel prize in physics\§ for their pioneering work showing

---

\*relative to, say, the electron mass
\†specifically, a left-handed chirality preference
\‡it would take infinite energy to make a massive particle travel at the speed of light, therefore only massless particles can travel at $c$. But, said particles experience no time or distance in their rest frame.
\§on behalf of the SNO and Super-Kamiokande Collaborations respectively
3.2. From Two Neutrinos to None

that neutrino flavours oscillate [91, 92], and hence that the neutrino has a non-zero mass.

All these discoveries have solidified the fact that neutrino physics requires theoretical developments BSM. Hence, if $0\nu\beta\beta$ requires a massive neutrino in order to happen, this alone is enough to make the statement that $0\nu\beta\beta$ is BSM. It so happens that the neutrino indeed must have mass for $0\nu\beta\beta$ to occur, for similar reasons that it requires mass to oscillate between flavours. We know (from the previous question) that $0\nu\beta\beta$ requires the neutrino to be its own anti-particle. The only difference between such a neutrino and its anti-particle partner is that one is left-handed and the other is right-handed. This flip in chirality can be achieved by viewing this neutrino in non-trivially different reference frames, and hence it needs mass.* This is why the discovery of neutrino oscillations has generated much excitement regarding the possibility of seeing $0\nu\beta\beta$.

\[ \text{In conclusion, the answer to the title of this sub-section is: true.} \]

Would $0\nu\beta\beta$ confirm that: The neutrino is a Majorana particle?

In 1937 [93], Ettore Majorana proposed a theory of a massive spin-$1/2$ particle which is its own anti-particle, in an attempt to rid of the seemingly unsatisfactory interpretation of a Dirac sea of negative energy holes. His equation comes out to

\[ \text{In relativity, a particle travelling at } c \text{ in one reference frame travels at } c \text{ in all reference frames. Thus, if a particle is massless (and therefore travels at speed } c \text{) then it cannot change chirality.} \]

---

*In relativity, a particle travelling at $c$ in one reference frame travels at $c$ in all reference frames. Thus, if a particle is massless (and therefore travels at speed $c$) then it cannot change chirality.
3.2. From Two Neutrinos to None

\[ i\dot{\psi} - m\psi_c = 0 \]  
(3.15)

where \( \phi \equiv \gamma^\mu \partial_\mu \) (using Einstein summation convention) and \( \gamma^\mu \) are the well-known gamma matrices. \( \psi_c \) is the “charge conjugate” of the four-component spinor, \( \psi \), defined by

\[ \psi_c \equiv C\bar{\psi}^T = C(\psi^\dagger \gamma^0)^T = C\gamma^0\psi^* \]

where \( C \) is the charge conjugation matrix. Upon the identification that

\[ \psi = \psi_c \]  
(3.16)

it is clear that the “Majorana equation” in (3.15) reproduces the Lorentz invariant physics of the Dirac equation for an electrically neutral field

\[ (i\phi - m)\psi = 0 \]

Particles that satisfy Equation (3.15) and (3.16) are their own anti-particles, by construction, and are referred to as “Majorana particles.” In summary,

**Remark 3.1**

If a particle is Majorana \( \implies \) it is its own anti-particle.

This implication has made the term “Majorana particle” synonymous with “a particle which is its own anti-particle.” However, one may ask: is the converse of Remark 3.1 necessarily true? That is, could there exist an equation which is Lorentz covariant and reproduces the quantum physics of a neutral particle being its own anti-particle, but that does not take on the form of Equation (3.15) and (3.16)? In a related vain, could a particle exist which obeys Equation (3.15), but does not satisfy Condition (3.16), and would it be called “Majorana”? And furthermore, if we allow for LNV (as we must for 0\( \nu \beta \beta \)), then why should one believe that minimal alterations to the Standard Model describe 0\( \nu \beta \beta \), as opposed to more drastic revisions to QFT itself? From the understanding of the author, there are currently no satisfactory answers to these questions, likely because the converse of Remark 3.1 has been put in place by convention.

From the previous discussion, it is acceptable that we must admit the neutrino is its own anti-particle in order for 0\( \nu \beta \beta \) to occur. And, disregarding the logical non-equivalence of Remark 3.1, many arguments have been constructed showing that the exchange neutrino must indeed be Majorana. The most noteworthy of these arguments is dubbed the “Schechter-Valle Theorem” [94]. Many would cite the blackbox developed by [94], reproduced in Figure 3.5 below, as definitively answering the title of this sub-section as: true. In essence, Schechter and Valle showed that a Majorana mass term of the neutrino is generated, by assuming only that: crossing symmetry holds in the weak interaction mediated by some “natural” local gauge theory, i.e., a cancellation of Figure 3.5 (e) would require an unnatural fine tuning of the physical parameters; the electron and up/down quarks are massive, as they certainly are; and the standard left-handed weak interaction holds, as in Equation (3.17) below [95]. Additionally, [96] and [97]
3.2. From Two Neutrinos to None

nearly simultaneously came to the same conclusions as Schechter and Valle, whilst also proving that $0\nu\beta\beta$ cannot happen via Dirac neutrinos.

$$\left(\bar{\nu}_e\gamma_{\mu}\nu_e + \bar{\nu}_d\gamma_{\mu}\nu_d\right)W^\mu \quad (3.17)$$

However, recent reviews of the literature have compiled a list of many alternate $0\nu\beta\beta$ mechanisms [48, 53, 70]. In fact, soon after the publication of the Schechter-Valle Theorem, proposals of supersymmetric theories have been made explaining $0\nu\beta\beta$ which “do not involve the exchange of Majorana neutrinos.” [98] Furthermore, a general quantitative analysis has been done by [95] which concludes that the blackbox analysis is insufficient, and leaves room for other contributions to the neutrino mass. These suggestions highlight the fact that once we admit that $0\nu\beta\beta$ requires physics BSM, we no longer have a conclusive grasp on what mediates the neutrinoless part of this decay. Could it be, then, that $0\nu\beta\beta$ can still happen without the requirement that the neutrinos are Majorana? And what experiments analyzing neutrinos could definitively establish the Dirac/Majorana/other nature of the neutrino? These are questions that the author believes warrants more discussion and scrutiny, despite current claims within the community that a positive measurement of $0\nu\beta\beta$ confirms that neutrinos are indeed Majorana [99–101].

With this said, theorists and experimentalists should not fret, since the discovery of $0\nu\beta\beta$
would still underline the need for significant changes to the Standard Model. But, if we cannot definitively say that a positive measurement of $0\nu\beta\beta$ would prove that the neutrino is Majorana, then what new physics can be concluded from it exactly? As described in the previous questions above, $0\nu\beta\beta$ would require a massive neutrino and LNV, both of which make it a BSM decay. We stress that these discoveries alone would be worthy of a Nobel prize in physics.

implies In conclusion, the question in the title of this sub-section is: (arguably) misleading.

Would $0\nu\beta\beta$ require quenching?

From the discussion in Section 3.1.4, a major concern for researchers studying $0\nu\beta\beta$ is: given $M^{2\nu}$ are quenched in the nuclear structure model used, should $M^{0\nu}$ also be quenched in that context? [53] The answer to this question is still very unclear. However, as we will see, since the closure approximation will be used for the $M^{0\nu}$ two-body matrix elements (whereas in Equation (3.7) it was not) the operator structure within the matrix elements completely changes. Thusly, perhaps $M^{0\nu}$ should not be quenched whatsoever. As stated previously, in this research we will only present unquenched results.

implies Overall, the answer to the title of this sub-section is: (currently) inconclusive.

3.3 Neutrinoless Double-Beta Decay

Neutrinoless double-beta decay came into the limelight quickly after the proposal of its neutrinoful counterpart, since early theoretical predictions* suggested its lifetime was much shorter than $2\nu\beta\beta$ [55]. Experimentally, it was expected that the neutrinoless version would be found first [58]. Now we understand that this is not the case, but $0\nu\beta\beta$ is still an exciting prospect (see Section 3.2 directly above). In particular, due to Equation (3.18) and (3.19) mentioned below, $0\nu\beta\beta$ has far reaching implications for the neutrino mass hierarchy scenarios (degenerate, normal, or inverted) [99].† Overall, neutrinoless double-beta decay indeed represents a massive undertaking for both the nuclear/particle experimental and theoretical communities.

3.3.1 Current Experimental Status for $0\nu\beta\beta$

The hunt for the first direct measurement of $0\nu\beta\beta$ is fast-paced and constantly evolving [53, 58]. The same nuclei which are candidates for $2\nu\beta\beta$, as listed in Section 3.1.1, are also candidates for $0\nu\beta\beta$. Hence, the main differences (detector type, location, sensitivity, etc) between double-beta decay experiments are decided by what nuclear source is chosen. To distinguish between a confirmation of $2\nu\beta\beta$ and $0\nu\beta\beta$, one uses the detected $Q$-value of the electron emission, see for instance Figure 10 of [53]. To date, $0\nu\beta\beta$ has never been definitively confirmed.

---

*At this time, parity violation had not been discovered, which significantly altered the $T_{1/2}$ estimates.
†For $0\nu\beta\beta$, experimentalists are currently on the edge of probing the inverted region [102].
3.3 Neutrinoless Double-Beta Decay

A curious point to note, though, is that in 2001, after extensive searches [103], $0\nu\beta\beta$ was claimed to have been found in $^{76}\text{Ge}$ by a subset of the Heidelberg-Moscow Collaboration [104]. This claim generated excitement, but it was subsequently scrutinized to the point that the current community does not accept its results [53, 105, 106]. In fact, many members of the collaboration came out to rebuke the prior publication [107], since they felt that the statistical analysis was incomplete, despite the persistence of the original proponents in the group [108]. Furthermore, many experiments like [109] have not been able to reproduce the supposed Heidelberg-Moscow measurement. This “Heidelberg-Moscow controversy” highlights the need for continuing experimental progress in the search for $0\nu\beta\beta$; both so that detector technologies can be advanced, and theoretical methods can be benchmarked against data.

Since the existence of the neutrinoless mode has not been established, many modern experiments are underway, such as [62, 100, 102, 110–112] among others [53]. But how do experimentalists know what sensitivities are required of their apparatus, in order to measure $0\nu\beta\beta$ for their nuclei of interest? The answer is that many of them take estimates from phenomenological studies. However, it is well known that the spread in NME calculations from competing methods is inconsistent, and theoretical uncertainties are currently out of reach [13]. So, in conjunction with the importance of experimental data in theoretical studies, in turn, theorists currently carry the responsibility to make accurate predictions of $0\nu\beta\beta$ NMEs for the sake of experimentalists. In this dissertation, we’ll calculate these NMEs using a fully ab initio approach called IM-SRG (see Chapter 5).

3.3.2 $0\nu\beta\beta$ Half-Life Formula

To move forward, we’ll now make the following assumption:

**Assumption 1**

The $0\nu\beta\beta$ mode occurs via the Majorana nature of neutrinos.

The original analysis of this mechanism was explored in [65]. An in-depth review of the $V-A$ particle physics and QFT involved can be found in [66], where they derive the half-life formula

$$[T_{1/2}^{0\nu}]^{-1} = G^{0\nu}|M^{0\nu}|^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2$$  \hspace{1cm} (3.18)

where $G^{0\nu}$ is known as the $0\nu\beta\beta$ “phase factor,” which incorporates the interface between particle and nuclear physics, and will be discussed more below; $M^{0\nu}$ is the NME, which incorporates nuclear structure theory (see Section 3.3.3 below); Equation (3.18) indeed obeys (F11), as expected; $m_e$ is the electron mass, and the “(effective) Majorana neutrino mass” is

$$\langle m_{\beta\beta}\rangle = \left|\sum_{k=1}^{3} m_k U_{ek}^2\right|$$  \hspace{1cm} (3.19)

where $U_{ek}$ are the first (aka, electron neutrino) row elements of the PMNS matrix, and $m_k$ are
the corresponding mass eigenstate neutrino masses. Equation (3.19) ties in the BSM physics involved with $0\nu\beta\beta$, hence Equation (3.18) bridges: QFT, BSM physics, and nuclear theory.

For us, this half-life formula is the prime motivator for the research conducted in this thesis project. To illuminate this, it is more appropriate to rewrite Equation (3.18) as

$$\langle m_{\beta\beta} \rangle = \frac{m_e}{\sqrt{G^{0\nu}_{1/2}[M^{0\nu}]}}$$  \hspace{1cm} \text{(3.20)}$$

Now we can see the rub! If the experimental physics community can measure the PMNS matrix precisely,* and make a measurement of the neutrinoless double-beta decay half-life $T^{0\nu}_{1/2}$ (see Section 3.3.1 above); and if the theoretical community can determine the value of the phase factor, and the NME; then one can determine the absolute mass scale of the neutrino. Viewing Equation (3.18) in the form of (3.20) is indicative of the model that Figure 3.5 (e) above acts as a Majorana neutrino mass contribution, via $0\nu\beta\beta$. Furthermore, since the decay is expected to be very rare and so $T^{0\nu}_{1/2}$ is large, this Majorana theory of the neutrino mass could explain why the neutrino has such a small mass [88, 94].

Making an accurate model of the NME is what we will focus on for the rest of this dissertation. Before we move on, however, it is important to stress, once again, that all this relies on the assumption that neutrinos are Majorana! As discussed in Section 3.2 above, this need not be the case. It could very well be that $0\nu\beta\beta$ exists and is dominated by a BSM mechanism not involving Majorana neutrinos, and the determination of Equation (3.20) is simply a soft prediction. Thus, it is important that the experimental community does not come to the immediate conclusion: a positive measurement of $0\nu\beta\beta \Rightarrow$ the neutrino is Majorana. Importantly, if it is the case that Equation (3.19) can be established numerically by alternative experiments, and combining this number into Equation (3.18) happens to match precisely with a confirmed measurement of the $0\nu\beta\beta$ half-life, only then it is likely that the neutrino is Majorana. This bold conclusion is reliant on having good $0\nu\beta\beta$ NMEs!

**$0\nu\beta\beta$ Phase Factor**

We’ll treat the neutrinoless phase factor in the same manner that we did for the two-neutrino case (see Section 3.1.2) - as a black box. Cowell was one of the first to notice that the phase factor had previously been treated inconsistently in the literature [114], which has now set a president for their modern calculation [67, 68]. For the sake of comparison† with Equation (3.4), [67] reports the $0\nu\beta\beta$ phase factor for $^{48}\text{Ca}$ as

$$G^{0\nu}(^{48}\text{Ca}) = 2.481 \times 10^{-14} \text{ yr}^{-1}$$

which is generally agreed upon [69].

---

*which is being done continually by neutrino oscillation experiments [113]

†Note that this comparison is contrived, since the structure of Equation (3.3) is different from that in (3.18), and the NMEs in either scenario are not necessarily comparable.
3.3. Nuclear Matrix Elements

The NME, $M^{0\nu}$, from Equation (3.18) may be decomposed into three dominate parts \[115\]

$$M^{0\nu} = M_{GT}^{0\nu} - \left( \frac{g_N}{g_A} \right)^2 M_F^{0\nu} + M_T^{0\nu} \tag{3.21}$$

This is very similar to $M^{2\nu}$ in Equation (3.6), except with an additional “Tensor” (T) part. This component has been induced specifically by the physics of neutrinoless double-beta decay. The derivation of this part can be found in \[66\] up to their Equation (3.5.7). There they considered two additional effects, being: alternate electron $P$-wave effects, and nucleon recoil. However, as is common with current trends in the literature, we will neglect these effects \[69\].

Note that in the notational convention of Equation (3.21), the GT, F, and T components of $M^{0\nu}$ may each carry a sign (they have not been written as magnitudes). It will be found that $M_{GT}^{0\nu}$ comes out positive, $M_F^{0\nu}$ comes out negative, and $M_T^{0\nu}$ comes out negative (see Section 7.2). Hence, the negative in front of $M_F^{0\nu}$ in Equation (3.21) will tend to cancel, whereas the induced negative from $M_T^{0\nu}$ will decrease the total sum. They are also written in order of largest to smallest in magnitude from left to right. In other words, it is common to find that

$$|M_{GT}^{0\nu}| > |M_F^{0\nu}| > |M_T^{0\nu}|$$

therefore many authors will simply neglect the Tensor part \[72, 116, 117\]. In this research, however, all three components will be analyzed, for completeness.

Now, how can we calculate each component of Equation (3.21)? First note that the NMEs are written in shorthand such that

$$M_{\alpha}^{0\nu} \doteq \langle f | \hat{M}_{\alpha}^{0\nu} | i \rangle \tag{3.22}$$

where, in the RHS, $|i\rangle$ is the state of the initial nuclei in the neutrinoless double-beta decay, likewise $|f\rangle$ is the state of the final nuclei, and $\hat{M}_{\alpha}^{0\nu}$ is the scalar spherical tensor operator representing $0\nu\beta\beta$ for $\alpha = GT$, F, or T. The reason these spherical tensors are scalar is simple. Let’s consider the Fermi component; from Section 2.3.2 we know this happens for a single-beta decay when the neutrino and beta particle are anti-aligned, and hence spin couples to 0. For two beta decays, then, total angular momentum must couple to 0 as well, and we know that spherical tensors can only change angular momentum in steps of their rank.* Hence, due to the selection rules of $0\nu\beta\beta$,† its spherical tensors are rank 0. To obtain values for Equation (3.22), we therefore need to find the scalar TBMEs for $0\nu\beta\beta$ and the corresponding TBTDs, in accordance with Equation (C33). The latter task will be dealt with using nutbar (see Section 6.3), and the former will be discussed in full detail in Chapter 4.

---

*This can be seen clearly when considering Equation (B14), for instance

†Also note that only spherical tensors of the same rank may be summed together, as in Equation (3.21).
3.3. Neutrinoless Double-Beta Decay

3.3.4 The Closure Approximation

Notice that, in the paragraph above, we referred to Equation (C33) as opposed to (C30) to compute values for (3.22). This is because we will employ the so-called closure approximation for $0\nu\beta\beta$. [118] showed that the difference between using the closure energy (see Equation (4.9) and Assumption 2 below) for $0\nu\beta\beta$, and using a non-closure method, is about 10% for the final NMEs. Furthermore, it is well known that varying the closure energy yields only small differences in the final values. With this knowledge, it is justified to compare NMEs which use a different value for the closure energy - and many authors adhere to different conventions.* Establishing which closure energy is optimal for the nuclei undergoing $0\nu\beta\beta$ decay will be left for future research.

*For example, 0.5 MeV or 7.72 MeV are both acceptable values for the $^{48}$Ca closure energy.


Chapter 4

$M^{0\nu}$ Two-Body Matrix Elements

In this chapter, we will present the mathematical construction of the $M^{0\nu}$ TBMEs, in full detail. First, recall from Equation (3.21) and (3.22) in Section 3.3.3 above that

$$M^{0\nu} = M^{0\nu}_{\mathrm{GT}} - \left(\frac{g_N}{g_A}\right)^2 M^{0\nu}_F + M^{0\nu}_T$$

where,

$$M^{0\nu}_\alpha = \langle f | \hat{M}^{0\nu}_\alpha | i \rangle, \quad \alpha = \mathrm{GT}, \ F, \ T \quad (3.22)$$

The individual NMEs of Equation (3.22) may be calculated using Equation (C33) and Equation (B9). That is, with spherical tensor rank $L = 0$, we have

$$\langle f | \hat{M}^{0\nu}_\alpha | i \rangle = \sum_{abcd \ J J'} \sum_{\eta J} \langle ab | J \rangle \left[ [\tilde{c}^\dagger_c \otimes \tilde{c}^\dagger_d] J \otimes [\tilde{c}_a \otimes \tilde{c}_b] J' \right] \langle \eta | J \rangle \langle \eta | J' \rangle \quad (4.1)$$

To calculate the TBTDs (see Section C.3) in Equation (4.1), we will use a code called nutbar (see Section 6.3). Before we may compute these NMEs fully, an essential component are the TBMEs, which will be denoted by the shorthand

$$M^{0\nu}_{\alpha \ abcd} \equiv \langle ab | J \rangle \hat{M}^{0\nu}_\alpha | cd \rangle, \quad \alpha = \mathrm{GT}, \ F, \ T \quad (4.2)$$

where $a, b, c, d$ represent all the relevant quantum numbers to describe the two-body states in $J$-scheme with $jj$-coupling (see Section A.1). That is, we have $\Delta(j_a j_b : J)$ and $\Delta(j_c j_d : J')$.

4.1 Deconstructing $M^{0\nu}$

We begin our long dive into the TBMEs of $0\nu\beta\beta$ by specifying what each scalar spherical tensor operator, $\hat{M}^{0\nu}_\alpha$, in Equation (4.2) represents. From the involved derivations of [64, 66], we obtain

$$\hat{M}^{0\nu}_{\mathrm{GT}} = H_{\mathrm{GT}}(r_{12}, E_k) y_{\mathrm{GT}}(\tilde{r}_{12}) \tilde{\sigma}_1 \cdot \tilde{\sigma}_2 \tau_1^+ \tau_2^+ \quad (4.3)$$

$$\hat{M}^{0\nu}_F = H_F(r_{12}, E_k) y_F(\tilde{r}_{12}) \tau_1^+ \tau_2^+ \quad (4.4)$$

$$\hat{M}^{0\nu}_T = H_T(r_{12}, E_k) y_T(\tilde{r}_{12}) \tilde{S}_{12} \tau_1^+ \tau_2^+ \quad (4.5)$$

where operators denoted by a subscript 1 (or 2) are meant to act on the first (or second) particle.

\*the spherical tensors for $0\nu\beta\beta$ must be scalar, as explained in Section 3.3.3
of a two-body state, and the \( y(\vec{r}) \)'s carry the obviously required spherical harmonic dependance, as in Equation (F7), via

\[
y_\alpha(\vec{r}_{12}) = \begin{cases} 
\sqrt{3\pi} Y_{00}(\vec{r}_{12}) = 1, & \alpha = \text{GT}, \text{F} \\
\sqrt{\frac{2\pi}{3}} Y_{2m}(\vec{r}_{12}), & \alpha = \text{T}
\end{cases} \quad (4.6)
\]

The isospin operators, \( \tau^+ \), simply act to transform a nucleon from a neutron state to a proton state, in accordance with the two beta decays. For the Tensor component, we have introduced the “tensor spin operator,” which is defined by

\[
\hat{S}_{12} \equiv 3(\vec{\sigma}_1 \cdot \vec{r}_{12})(\vec{\sigma}_2 \cdot \vec{r}_{12}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2 \rightarrow [\vec{\sigma}_1 \otimes \vec{\sigma}_2]_2 \quad (4.7)
\]

where,

\[
\vec{r}_{12} \equiv \vec{r}_1 - \vec{r}_2, \quad r_{12} \equiv ||\vec{r}_{12}||, \quad \hat{r}_{12} \equiv \frac{\vec{r}_{12}}{r_{12}} \quad (4.8)
\]

The relative coordinate, \( \vec{r}_{12} \), tracks particle 1 and 2, before second quantization. That is, for the final TBMEs, \( r_{12} \) will be integrated over with respect to the appropriate probability amplitudes and spherical harmonics. It is in conjunction with this spacial integration that the mapping on the RHS of Equation (4.7) occurs; that is, the tensor spin operator, \( \hat{S}_{12} \), becomes a rank 2 spherical tensor product between two Pauli operators. Likewise, the spherical harmonics of Equation (4.6) will also be treated as spherical tensors, as we will see in Equation (4.21) below.

The \( H_\alpha \)'s in Equations (4.3) to (4.5) are known as “neutrino potentials,” which are integrals over the neutrino exchange momentum, \( q \), and they depend on the energy of the intermediate state \( k \) of the neutrinoless double-beta decay. In their most general form, they are written as

\[
H_\alpha(r_{12}, E_k) = \frac{2R}{\pi} \int_0^\infty dq \frac{q^2 f_\alpha(q \cdot r_{12})h_\alpha(q^2)}{\omega[q^2 + (E_i + E_f)/2]} \quad (4.9)
\]

where \( r_{12} \) is the same as in Equation (4.8), \( R \) is the nuclear radius given by (2.29), \( \omega \) is the neutrino energy given by \( \omega = \sqrt{q^2 + m_\nu^2} \), and the functions, \( f_\alpha(q \cdot r_{12}) \), are defined simply as

\[
f_\alpha(q \cdot r_{12}) = \begin{cases} 
\begin{align*}
j_0(q \cdot r_{12}), & \alpha = \text{GT, F} \\
j_2(q \cdot r_{12}), & \alpha = \text{T}
\end{align*}
\end{cases} \quad (4.10)
\]

where the \( j(x) \)'s are spherical Bessel’s functions as in Equation (F5). The functions, \( h_\alpha(q^2) \), are the finite-size“(nucleon) form factors,” which are listed below

\[
h_\text{F}(q^2) \equiv \frac{g_\text{F}^2(q^2)}{g_{V,0}} \quad (4.11)
\]

\[
h_{\text{GT}}(q^2) \equiv \frac{1}{g_{A,0}^2} \left[ g_A^3(q^2) - \frac{g_A(q^2)g_P(q^2)q^2}{3m_p} + \frac{g_P^2(q^2)q^4}{12m_p^2} + \frac{g_M^2(q^2)q^2}{6m_p^2} \right] \quad (4.12)
\]
4.1. Deconstructing $M^{0\nu}$

\[
h_T(q^2) = \frac{1}{g_{A,0}^2} \left[ \frac{g_A(q^2) g_P(q^2)}{3m_p} q^2 - \frac{g_P^2(q^2) q^4}{12m_p^2} + \frac{g_M^2(q^2) q^2}{12m_p^2} \right]
\]

\[
\equiv \frac{g_A^2(q^2)}{g_{A,0}^2} \left[ \frac{2}{3} \frac{q^2}{q^2 + m_{\pi}^2} - \frac{1}{3} \left( \frac{q^2}{q^2 + m_{\pi}^2} \right)^2 \right] + \frac{1}{12} \frac{g_M^2(q^2) q^2}{g_{A,0}^2 m_p^2}
\]

(4.13)

with the vector ($V$), axial-vector ($A$), pion-exchange propagator ($P$), and magnetic moment ($M$)

“(regularized) $g$-factors” are as follows

\[
g_V(q^2) \equiv \frac{g_{V,0}}{(1 + q^2/\Lambda_V^2)^2}, \quad g_A(q^2) \equiv \frac{g_{A,0}}{(1 + q^2/\Lambda_A^2)^2}
\]

\[
g_P(q^2) \equiv \frac{2m_p g_A(q^2)}{q^2 + m_{\pi}^2}, \quad g_M(q^2) \equiv \left( \frac{\mu_p - \mu_n}{\mu_N} \right) g_V(q^2)
\]

(4.14)

and the proton mass $m_p$, pion mass $m_{\pi}$, “(finite-size) cutoffs” $\Lambda$, and magnetic moment $\mu_p, \mu_n, \mu_N$ values will be specified when the NMEs are calculated.

There are two glaring points to make about the neutrino potentials before we move on.

First, we will impose some approximations on the general form of Equation (4.9). It’s clear that the neutrino mass is small [119], and hence: $\omega \approx q$, by taking $q \gg m_\nu$. Next, to guarantee that we may employ Equation (4.1), we must use the closure approximation (see Section C.3.1 and 3.3.4) so that $\hat{M}_0^{0\nu}$ is independent of $k$ via:

**Assumption 2: “The Closure Energy”**

In order to make the $0\nu\beta\beta$ operators of Equations (4.3) to (4.5) independent of the intermediate nuclear state, we impose the closure approximation by introducing the “closure energy”

\[
E_k + (E_i + E_f)/2 \approx E_{0}^{\text{cl}}
\]

(4.15)

For now, we’ll assume that this approximation holds, since [118] showed that varying the closure energy only introduces small changes to the overall NME.

Choosing the best closure energy seems to depend on the parent nucleus of the neutrinoless double-beta decay [118]; more on this should be explored in future research. Putting Equation (4.15) and $\omega \approx q$ into (4.9) gives us the more computationally manageable neutrino potentials

\[
H_\alpha(r_{12}, E_k) \rightarrow H_\alpha(r_{12}) = \frac{2R}{\pi} \int_0^\infty dq \frac{q \cdot f_\alpha(q \cdot r_{12}) h_\alpha(q^2)}{q + E_0^{\text{cl}}}, \quad \alpha = \text{GT, F, T}
\]

(4.16)

It is evident that Equation (4.16) above behaves as a Yukawa potential in $r_{12}$ [66].

Secondly, the nuclear radius, $R$, has been included to make the neutrino potentials unitless, but this yields some confusion within the nomenclature. That is, the physics of neutrinoless double-beta decay itself should, intuitively, be independent of the nucleus of interest. But, with the inclusion of $R$, this will make the $0\nu\beta\beta$ NMEs *nuclei-dependent*. This makes combining the
4.2 Tensor TBMEs

NME with phase factors* of Equation (3.18) more convenient. Thus, even though \( \hat{M}_0^{0\nu} \) should only be \( 0\nu\beta\beta \)-dependant, and \( M_{abcd}^0 \) of Equation (4.2) are nuclear structure dependant; due to the current literature conventions, both are nuclei-dependant.

One final point to make in deconstructing \( M_0^{0\nu} \) is that we will deal with isospin in the “PN” formalism. That is, the projected isospin† of our nucleon states will be well-defined. Therefore, we’ll separate out the isospin component from the operators, \( \hat{M}_0^{0\nu} \), before any coupling or reduction of the TBMEs in Equation (4.2). So each operator structure in Equations (4.3) to (4.5) will yield a prefactor of

\[
\langle t_a, t_b | r_1^+ r_2^+ | t_c, t_b \rangle = \langle t_a | t_c + 1 \rangle \langle t_b | t_d + 1 \rangle = \delta_{t_a, t_c + 1} \delta_{t_b, t_d + 1} \equiv \delta^{iso}_{ac,bd}
\]  

(4.17)

When the Kronecker-delta in Equation (4.17) appears, it should be understood that the isospin quantum numbers have been separated from \( a, b, c, d \) for (4.2). It can be easily seen that, physically, this Kronecker-delta represents the transformation of two neutrons to two protons, in accordance with the double-beta decay.

4.2 Tensor TBMEs

We’ll begin with the most complicated structure; that of the Tensor component of the \( M_0^{0\nu} \) TBMEs. Using Equations (4.2), (4.5), (4.17), and (4.16) we get

\[
M^T_{abcd} = \delta^{iso}_{ac,bd} \langle a b : J || H_T (r_{12}) y_T (\hat{r}_{12}) \tilde{S}_{12} || c d : J' \rangle \\
= \delta^{iso}_{ac,bd} \frac{2 R}{\pi} \int_0^\infty dq \frac{q \cdot h_T(q^2)}{q + E_{cl}^0} \langle a b : J || f_T (q \cdot r_{12}) y_T (\hat{r}_{12}) \tilde{S}_{12} || c d : J' \rangle
\]  

(4.18)

Note that in Equation (4.18) we retained \( f_T \) and \( y_T \) within the reduced matrix elements, since they are coordinate-dependant and therefore must be integrated over via the product of two-body states. We pulled the integral with respect to the neutrino exchange momentum, \( q \), outside of the states since - due to the structure of the form factors in Equations (4.11) to (4.13) - we will need to handle the integration numerically. This complicates matters, in that each reduced matrix element will need to be integrated individually (see Section 6.4 for more details); but it balances out, since the integration with respect to the states can be done analytically (see Section 4.5 below). To simplify the notation, let’s define the augmented operator

\[
\hat{Q}_T \equiv f_T (q \cdot r_{12}) y_T (\hat{r}_{12}) \tilde{S}_{12}
\]  

(4.19)

which we labelled as a “\( \hat{Q} \)” to remind us that it has \( q \)-dependence.

Now we must deal with the elements \( \langle a b : J || \hat{Q}_T || c d : J' \rangle \), but how? The trick is to notice that we must transform from \( jj \)-coupling to \( ls \)-coupling, as to clarify the operator’s action on the spin quantum numbers. From that point on, the Talmi-Moshinsky transformation of Section 2.1.2 can be used to resolve the relative radial coordinate dependence. Using Equation (A34) gives

---

*which are nuclei-dependant, by construction
†proton with \( t_z = +1/2 \) and neutron with \( t_z = -1/2 \), see Section 2.2.1
\begin{align*}
||cd:J'|| = ||(l_c \frac{1}{2} j_c, (l_d \frac{1}{2} j_d):J') = \sum_{LL'S'} \left[ \begin{array}{ccc}
l_c & l_d & L' \\
\frac{1}{2} & \frac{1}{2} & S' \\
j_c & j_d & J'
\end{array} \right] \|||(l_d l_d)L', (\frac{1}{2} \frac{1}{2})S':J')
\end{align*}

and likewise for \( \langle ab:J|| \). Using the above re-coupling, and Equation (4.19), we may write
\[
\langle ab:J||\hat{Q}_T||cd:J'\rangle = \sum_{LL'S'} \sum_{SS'} \left[ \begin{array}{ccc}
l_a & l_b & L \\
\frac{1}{2} & \frac{1}{2} & S \\
j_a & j_b & J
\end{array} \right] \left[ \begin{array}{ccc}
l_c & l_d & L' \\
\frac{1}{2} & \frac{1}{2} & S' \\
j_c & j_d & J'
\end{array} \right] \langle LS:J||\hat{Q}_T||L'S':J'\rangle \quad (4.20)
\]

In this form it is clear that the spherical harmonics will act on the total orbital angular momentum quantum numbers of our two-body states, whereas the \( \hat{S}_{12} \) will act on the total spin.

We may now treat \( y_T \) within \( \hat{Q}_T \) as carrying spherical tensor harmonic structure. Hence, through Equations (4.6), (4.10), and (4.7), we take the operator inside of (4.20) as a scalar product (see Definition B.5) between the two rank 2 spherical tensors, such that
\[
\hat{Q}_T = f_T(q\cdot r_{12})y_T(\hat{r}_{12})\hat{S}_{12} \rightarrow \sqrt{\frac{24\pi}{5}} [j_2(q\cdot r_{12})\hat{Y}_2(\hat{r}_{12})]_{12} [\vec{\sigma}_1 \otimes \vec{\sigma}_2]_2 \quad (4.21)
\]

Then using Equation (B16) of Corollary B.2.1 with (4.21) yields
\[
\langle LS:J||\hat{Q}_T||L'S':J'\rangle = \delta_{JJ'}(-1)^{S+J+L'} \left\{ \begin{array}{ccc}
L & S & J \\
S' & L' & 2
\end{array} \right\} 
\times \sqrt{\frac{24\pi}{5}} \langle L||j_2(q\cdot r_{12})\hat{Y}_2(\hat{r}_{12})||L'\rangle \langle S||[\vec{\sigma}_1 \otimes \vec{\sigma}_2]_2||S'\rangle \quad (4.22)
\]

From Equation (B15) of Theorem B.2, we see that
\[
\langle S||[\vec{\sigma}_1 \otimes \vec{\sigma}_2]_2||S'\rangle = \langle 1 \frac{1}{2} : S||[\vec{\sigma}_1 \otimes \vec{\sigma}_2]_2||1 \frac{1}{2} : S'\rangle = \hat{S} \hat{S}' \left\{ \begin{array}{ccc}
\frac{1}{2} & \frac{1}{2} & S \\
\frac{1}{2} & \frac{1}{2} & S'
\end{array} \right\} \langle 1 \frac{1}{2}||[\vec{\sigma}_1 ||1 \frac{1}{2}||[\vec{\sigma}_2 ||1 \frac{1}{2} \rangle
\]
\[
= 6\sqrt{5} \hat{S} \hat{S}' \left\{ \begin{array}{ccc}
\frac{1}{2} & \frac{1}{2} & S \\
\frac{1}{2} & \frac{1}{2} & S'
\end{array} \right\} \quad (4.23)
\]

where we used Equation (2.42) for the vector spherical tensor Pauli operators \( \vec{\sigma}_1 \) and \( \vec{\sigma}_2 \), each of rank 1. It’s clear that \( S = 0 \) or 1 since \( \Delta(\frac{1}{2} \frac{1}{2} : S) \), and likewise for \( S' \). Calculating the \( 9j \)-symbol from Equation (4.23) over this range of values for \( S \) and \( S' \) gives
\[
\left\{ \begin{array}{ccc}
\frac{1}{2} & \frac{1}{2} & S \\
\frac{1}{2} & \frac{1}{2} & S'
\end{array} \right\} = \begin{cases}
1/9, & S = S' = 1 \\
0, & \text{o.w.}
\end{cases}
\quad (4.24)
\]

and so, plugging Equation (4.24) into (4.23) with \( \hat{1} = \sqrt{3} \), yields
\[
\langle S||[\vec{\sigma}_1 \otimes \vec{\sigma}_2]_2||S'\rangle = 2\sqrt{5} SS' = \begin{cases}
2\sqrt{5}, & S = S' = 1 \\
0, & \text{o.w.}
\end{cases}
\quad (4.25)
\]

Equation (4.25) may seem innocuous, but it severely restricts the summation over \( S, S' \) in
Equation (4.20). That is, since the $9j$-symbol is zero unless $S = S' = 1$, we only need to consider these values and then sum over $L, L'$, which are coupled as $\Delta(l_a l_b; L)$ and $\Delta(l_c l_d; L')$ respectively. So, putting Equation (4.25) into (4.22), and the result into (4.20) gets

$$(ab:J||cd:J') = \sum_{LL'} 2\sqrt{5}(-1)^{1+J+L'} \begin{pmatrix} L & 1 & J \\ 1 & L' & 2 \end{pmatrix} \begin{pmatrix} l_a & l_b & L \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} l_c & l_d & L' \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix} \sqrt{\frac{24\pi}{5}} \langle L||j_2(q \cdot r_{12})\hat{Y}_2(r_{12})||L' \rangle$$

(4.26)

From here we note that the coordinate, $\hat{r}_{12}$ as defined in Equation (4.8), is measured radially, relative to particles 1 and 2. Thus, since $L$ and $L'$ are set in the lab frame, we must transform into the relative/CoM coordinates via the Talmi-Moshinsky transformation of Theorem 2.1 - in order to clarify the action of the rank 2 spherical tensor operator $j_2(q \cdot r_{12})\hat{Y}_2(r_{12})$ on the states. Using Equation (2.11), we obtain

$$\langle l_a, l_b; L||j_2(q \cdot r_{12})\hat{Y}_2(r_{12})||l_c, l_d; L' \rangle = \hat{L}' \sum_{n_{a},l_r,n'_{a},l'_r} D_{ab} D'_{cd} (-1)^{L'+l_r} \begin{pmatrix} L & l_r & \Lambda \\ l'_r & L' & 2 \end{pmatrix} \times \langle n_{a}, l_r; j_2(q \cdot r_{12})\hat{Y}_2(r_{12})||n'_{a}, l'_r \rangle$$

(4.27)

with the Talmi-Moshinsky brackets

$$D_{ab} = \langle n_{a}, l_r, NA:L||n_{a}, l_a, b, l_b; L \rangle \quad \text{and} \quad D'_{cd} = \langle n'_{a}, l'_r, NA:L'||n_{c}, l_c, n_d, l_d; L' \rangle$$

(4.28)

and the corresponding CTML from Equation (D21). A tricky caveat to point out about Equation (4.27) is that the relative/CoM coordinates used to construct the brackets are built as

$$\hat{r} = \frac{1}{\sqrt{2}} (\hat{r}_1 - \hat{r}_2) \quad \text{and} \quad \hat{R} = \frac{1}{\sqrt{2}} (\hat{r}_1 + \hat{r}_2)$$

(2.8)

Comparing this with Equation (4.8) introduces a factor of $\sqrt{2}$, which must be accounted for

$$\hat{r}_{12} = \sqrt{2}\hat{r} \implies r_{12} = \sqrt{2}r \quad \text{and} \quad \hat{r}_{12} = \hat{r}$$

(4.29)

Finally, we can separate out the action of the spherical Bessel’s function and the spherical harmonics using Equation (B14) of Example B.3. This with Equation (4.29) gives us

$$\langle n_r, l_r; j_2(q \cdot r_{12})\hat{Y}_2(r_{12})||n'_{r}, l'_r \rangle \approx \langle n_r, l_r; j_2(\sqrt{2}qr)\hat{Y}_2(r)||n'_{r}, l'_r \rangle = \sqrt{\frac{5}{4\pi}} (l_r \, 0 \, 2 \, 0 \, l'_r \, 0) \hat{l}_r \langle n_r, l_r; j_2(\sqrt{2}qr)||n'_{r}, l'_r \rangle$$

(4.30)

Plugging Equation (4.30) into (4.27), and the result into Equation (4.26) yields
\[ \langle a b: J || \hat{Q}_T || c d: J' \rangle = \delta_{J J'} \overline{J} \sum_{LL'} 2\sqrt{5} (-1)^{1+J+L'} \overline{L} \overline{L}' \left\{ \begin{array}{ccc} L & 1 & J \\ 1 & L' & 2 \end{array} \right\} \]
\[ \times \left[ \begin{array}{ccc} l_a & l_b & L \\ J_a & J_b & J \end{array} \right] \left[ \begin{array}{ccc} l_c & l_d & L' \\ J_c & J_d & J \end{array} \right] \]
\[ \times \sum_{n_r l_r, n'_r l'_r \leq N} D_{ab} D'_{cd} (-1)^{L'+l_r} \left\{ \begin{array}{ccc} L & l_r & \Lambda \\ l'_r & L' & 2 \end{array} \right\} \]
\[ \times \sqrt{6} (l_r 0 2 0 \, | \, l'_r 0) \langle n_r l_r | j_2 (\sqrt{2} q r) | n'_r l'_r \rangle \]

where \( \hat{Q}_T \) is defined in Equation (4.19), the sum over angular momentum runs as \( \Delta(l_a l_b : L) \) and \( \Delta(l_c l_d : L') \), the Talmi-Moshinsky brackets \( D_{ab} \) and \( D'_{cd} \) are defined in (4.28), and we may adapt Equation (D21) for our CTML. We’ll call the integrals over \( dr \) “relative Bessel’s matrix elements” (RBMEs), which can be calculated analytically; see Section 4.5 below.

### 4.3 Gamow-Teller TBMEs

The calculation of the Gamow-Teller component of the \( M^{ll}\overline{ll} \) TBMEs is similar to that of the Tensor component done in the section above, but it is somewhat simpler. Using Equations (4.2), (4.3), (4.17), and (4.16), we may write

\[ M_{abcd}^{GT} = \delta_{ac, bd} \frac{2R}{\pi} \int_0^\infty dq \frac{q \cdot h_{GT}(q^2)}{q + E_0^\Gamma} \langle a b: J || \hat{Q}_GT || c d: J' \rangle \]  
(4.32)

where, \( \hat{Q}_GT \equiv f_{GT}(q \cdot r_{12}) y_{GT}(\hat{r}_{12}) \hat{\sigma}_1 \hat{\sigma}_2 \)  
(4.33)

and \( f_{GT}, y_{GT}, \) and \( h_{GT} \) are defined in Equations (4.10), (4.6), and (4.12) respectively. As we did with the Tensor component, we’ll transform from \( jj \)-coupling to \( ls \)-coupling via

\[ \langle a b: J || \hat{Q}_GT || c d: J' \rangle = \sum_{LL'} \sum_{SS'} \left[ \begin{array}{ccc} l_a & l_b & L \\ \frac{1}{2} & \frac{1}{2} & S \end{array} \right] \left[ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & S' \end{array} \right] \left[ \begin{array}{ccc} l_c & l_d & L' \\ j_c & j_d & J' \end{array} \right] \langle LS: J || \hat{Q}_GT || L'S': J' \rangle \]  
(4.34)

Now we can promote the \( \hat{Q}_GT \) to spherical tensor operator status by taking the scalar product between two rank 0 operators as so

\[ \hat{Q}_GT = f_{GT}(q \cdot r_{12}) y_{GT}(\hat{r}_{12}) \hat{\sigma}_1 \hat{\sigma}_2 \longrightarrow \sqrt{4\pi} \langle j_0(q \cdot r_{12}) Y_0(\hat{r}_{12}) \rangle_0 \otimes [\hat{\sigma}_1 \hat{\sigma}_2]_0 \]  
(4.35)

\[ \langle LS: J || \hat{Q}_GT || L'S': J' \rangle = \delta_{L L'} \delta_{S S'} \delta_{JJ'} \frac{\hat{j}}{SL} \sqrt{4\pi} \langle L || j_0(q \cdot r_{12}) Y_0(\hat{r}_{12}) || L' \rangle \langle S || [\hat{\sigma}_1 \hat{\sigma}_2] || S' \rangle \]  
(4.36)

To obtain (4.36), we plugged Equation (4.35) into (B21) of Corollary B.2.2. Notice that we’ve omitted the triangular delta, \( \delta_{(LS,J)} \), since it is clear from the context of \( ls \)-coupling.

We could construct the analogous equation to (4.23) to find \( \langle S || [\hat{\sigma}_1 \hat{\sigma}_2] || S' \rangle \), or we could make use of a commonly employed trick from many-body quantum mechanics. From Equation (2.38),
4.3. Gamow-Teller TBMEs

in units of $\hbar = 1$, it’s clear that

$$\langle S|\vec{\sigma}_1 \cdot \vec{\sigma}_2|S'\rangle = 4\langle S|\vec{S}_1 \cdot \vec{S}_2|S'\rangle \quad (4.37)$$

Additionally, we can make use of knowing the eigenvalues of $\vec{S}^2$ via the following manipulation,

$$\vec{S}^2 = (\vec{S}_1 + \vec{S}_2)^2 = \vec{S}_1^2 + 2\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2^2 \implies \vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}[\vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2]$$

and hence the eigenvalues are

$$\vec{S}_1 \cdot \vec{S}_2 \rightarrow \frac{1}{2}[s(s + 1) - s_1(s_1 + 1) - s_2(s_2 + 1)] \quad (4.38)$$

For two spin-$1/2$ particles* the total spin (labelled as $s$ here) is coupled as

$$\Delta(s_1 = \frac{1}{2}, s_2 = \frac{1}{2} : s) \implies s = 0, 1 \quad (4.39)$$

Plugging Equation (4.39) into (4.38), and the result into (4.37) yields

$$\langle S|\vec{\sigma}_1 \cdot \vec{\sigma}_2|S'\rangle = \delta_{SS'} \cdot \sigma(S) \quad \text{where, } \sigma(S) \equiv 2S(S + 1) - 3 = \begin{cases} 1, & S = 1 \\ -3, & S = 0 \end{cases} \quad (4.40)$$

In analogy with Example B.2, using the Wigner-Eckhart Theorem (Theorem B.1), we can show that the reduced version of Equation (4.40) is

$$\langle S|\vec{\sigma}_1 \cdot \vec{\sigma}_2|S'\rangle = \delta_{SS'} \cdot \sigma(S) \quad (4.41)$$

Putting Equation (4.41) into (4.36) gives us

$$\langle LS:J||\hat{Q}_{GT}||L' S':J'\rangle = \delta_{LL'} \delta_{SS'} \delta_{J,J'} \cdot \hat{J} \cdot \sigma(S) \frac{\sqrt{4\pi}}{L} \langle L||j_0(q \cdot r_{12})\hat{Y}_0(\hat{r}_{12})||L'\rangle \quad (4.42)$$

As opposed to the case with the Tensor component, now we have a spherical tensor harmonic of rank 0 within our operator, and thus we can use the much simpler form of the Talmi-Moshinsky transformation presented in Corollary 2.1.1. Using Equation (2.20) gives

$$\langle l_a, l_b; L||j_0(q \cdot r_{12})\hat{Y}_0(\hat{r}_{12})||l_c, l_d; L'\rangle = \delta_{LL'} \cdot \tilde{J} \sum_{n_i l_i, n'_i} D_{ab}^{n'_i} D_{cd}^{n_i} \cdot \hat{r}^{-1} \langle n_r l_r||j_0(q \cdot r_{12})\hat{Y}_0(\hat{r}_{12})||n'_r l'_r\rangle \quad (4.43)$$

with the Talmi-Moshinsky brackets

$$D_{ab} = \langle n_r l_r, N \Lambda; L||n_a l_a, n_b l_b; L\rangle \text{ and, } D_{cd}^{n_i} \equiv \langle n'_r l'_r, N \Lambda; L||n_c l_c, n_d l_d; L\rangle \quad (4.44)$$

and the corresponding CTML from Equation (D16). Once again, using Equation (B14)

$$\langle n_r l_r||j_0(q \cdot r_{12})\hat{Y}_0(\hat{r}_{12})||n'_r l'_r\rangle = \frac{\hat{r}}{\sqrt{4\pi}} (l_r 0 0 0 | l_r 0) \langle n_r l_r||j_0(\sqrt{2}q r)||n'_r l'_r\rangle \quad (4.45)$$

where the CG coefficient goes to unity via Equation (A14), and we’ve again corrected for the discrepancy between the radial coordinate definitions for the Talmi-Moshinsky brackets using

---

*such as our nucleons
4.4. Fermi TBMEs

Equation (4.29). Inserting Equation (4.45) into (4.43), and the result into (4.42) and (4.34), whilst cancelling the appropriate hat factors and also summing over $L'$ and $S'$ produces

\[
\langle a b : J || \hat{Q}_{\text{GT}} || c d : J' \rangle = \delta_{J,J'} \sum_{S=0,1} \alpha \sigma (S) \left[ \sum_{L} \left[ \begin{array}{cc} l_a & l_b \frac{1}{2} \frac{1}{2} \\ \frac{1}{2} & S \\ \frac{1}{2} & \frac{1}{2} \end{array} \right] \right] \frac{L}{S} \frac{J}{J'} \frac{c_d | j_0 (\sqrt{2} q r) | n_r l_r \rangle}{\sqrt{4 \pi} \langle L || j_0 (q \cdot r_{12}) \hat{Y}_0 (\hat{r}_{12}) || L' \rangle} \]

(4.46)

where $\hat{Q}_{\text{GT}}$ is defined in Equation (4.33), the spin eigenvalues labelled by $\alpha \sigma$ are given in (4.40), the sum over angular momentum runs as $\Delta (l_a l_b : L)$ with the restriction that $\Delta (l_c l_d : L)$, the Talmi-Moshinsky brackets $D_{ab}$ and $D_{cd}^{n_r}$ are defined in (4.44), and we may adapt Equation (D16) for our CTML. The RBMEs can be calculated analytically; see Section 4.5 below.

4.4 Fermi TBMEs

The only part that differs between the operator structure of the Fermi component and the Gamow-Teller component of $M^{0\nu}$ is the presence of $\hat{\sigma}_1 \hat{\sigma}_2$. Therefore, to get the Fermi component, we may adapt Equation (4.35) and Equation (4.36) by replacing $\hat{\sigma}_1 \hat{\sigma}_2 \rightarrow 1$,

\[
\langle L S : J || \hat{Q}_{F} || L' S' : J' \rangle = \delta_{L,L'} \delta_{S,S'} \delta_{J,J'} \frac{J}{SL} \frac{4 \pi}{\sqrt{4 \pi}} \langle L || j_0 (q \cdot r_{12}) \hat{Y}_0 (\hat{r}_{12}) || L' \rangle \langle S || 1 || S' \rangle
\]

(4.47)

where

\[
M^{F}_{abcd} = \delta_{\text{iso}} \frac{2R}{\pi} \int_{0}^{\infty} dq \frac{q \cdot h_F (q^2)}{q + E^{cl}_0} \langle a b : J || \hat{Q}_{F} || c d : J' \rangle
\]

(4.48)

where, $\hat{Q}_{F} \equiv f_F (q \cdot r_{12}) y_F (\hat{r}_{12}) \mathbb{1}$

(4.49)

and $f_F, y_F,$ and $h_F$ are defined in Equations (4.10), (4.6), and (4.12) respectively. From Equation (B11), we see that

\[
\langle S || 1 || S' \rangle = \delta_{SS'} \hat{S}
\]

so plugging this into Equation (4.47), and repeating the identical math of Section 4.3 directly above yields the TBMEs of the Fermi component for $M^{0\nu}$

*for computational efficiency, where the 9j-symbols yield zero
where the sum over spin runs as $\Delta(\frac{1}{2} \frac{1}{2} : S)$, the sum over angular momentum runs as $\Delta(l_a l_b : L)$ with the restriction that $\Delta(l_c l_d : L)$, the Talmi-Moshinsky brackets $D_{ab}$ and $D_{cd}^\nu$ are defined in (4.44), and we may adapt Equation (D16) for our CTML. Below, we’ll calculate the RBMEs using an analytical integration.

### 4.5 Relative Bessel’s Matrix Elements

In this section we will follow the techniques laid out in [118] to find the analytic form of the relative Bessel’s matrix elements (RBMEs) appearing in Equations (4.31), (4.46), and (4.50)

$$
\langle a:b|J|c:d'\rangle = \delta_{J,J'} \sum_{L,S} \begin{bmatrix} l_a & l_b & L \cr \frac{1}{2} & \frac{1}{2} & S \cr j_a & j_b & J \end{bmatrix} \begin{bmatrix} l_c & l_d & L \cr \frac{1}{2} & \frac{1}{2} & S \cr j_c & j_d & J \end{bmatrix} \times \sum_{n_l,n_l'} D_{ab} D_{cd}^\nu (n_l, l_r | j_0(\sqrt{2qr}) | n_l', l_r')
$$

(4.50)

where $q$ is the momentum transfer of the Majorana neutrinos, $j_\rho$ are the spherical Bessel functions of order $\rho$ as in Equation (F5), and $R_{nl}(r)$ are the radial harmonic oscillator wavefunctions given by Equation (2.3). Notice that we’ve used the $r$ as in Equation (4.29), in order to match the radial oscillator wave-functions with our construction of the Talmi-Moshinsky brackets. With 20/20-hindsight, we will evaluate the (more grotesque) integrals

$$
\langle n_l l_r | W(q,r) | n_l' l_r' \rangle = \int_0^\infty dr r^2 R_{n_l l_r}(r) j_\rho(\sqrt{2qr}) R_{n_l' l_r'}(r)
$$

(4.51)

where $W(q,r) \equiv r^u e^{-wr^2} j_\rho(sqr)$ with $u, w, s \in \mathbb{R}$

and $u = 0 = w, s = \sqrt{2}$ retrieves our original integral. To solve Equation (4.52), let’s first make the notational simplification $n_r, l_r \rightarrow n, l$, and then plug the radial wave-functions

$$
\langle n l | W(q,r) | n' l' \rangle = \int_0^\infty dr r^{2+u} e^{-wr^2} j_\rho(sqr) N_{nl} N_{n'l'} \left( \frac{1}{b} \right)^{l+l'} e^{-r^2/2b^2} L_n^{l+\frac{1}{2}} (r^2/b^2) L_{n'}^{l'+\frac{1}{2}} (r^2/b^2)
$$

$$
= N_{nl} N_{n'l'} \left( \frac{1}{b} \right)^{l+l'} \int_0^\infty dr r^{l+l'+2+u} e^{-(\frac{1}{2b^2}+w)r^2} \times j_\rho(sqr) L_n^{l+\frac{1}{2}} (r^2/b^2) L_{n'}^{l'+\frac{1}{2}} (r^2/b^2)
$$

(4.53)

The $L$’s in Equation (4.53) are Laguerre polynomials, as in Equation (F3). Hence, we can use the well known fact that, for some $\alpha \in \mathbb{N}_0$ and $\beta \in \mathbb{R}$, we can expand them as follows

$$
L_\alpha^\beta(x) = \sum_{k=0}^{\alpha} \binom{\alpha + \beta}{\alpha - k} \frac{(-x)^k}{k!}
$$

(4.54)
where the coefficient in the sum is a generalized binomial coefficient, as defined in Equation (F2).

Using the expansion in Equation (4.54) for both the Laguerre polynomials in (4.53) gives

\[
\langle n|W(q, r)|n'\rangle = N_{nl}N_{n'l'}\left(\frac{1}{b}\right)^{l+l'} \int_0^\infty dr \, r^{l+l'+2+u} e^{-\frac{(r^2+w)}{2}} \int_0^\infty dr \, r^{l+l'+2+u} e^{-\frac{(r^2+w)}{2}} \int_0^\infty dr \, r^{l+l'+2+u} e^{-\frac{(r^2+w)}{2}}
\]

Applying Equation (E16) to the equation above, and staying consistent with the identifications in Equation (4.56) and (4.57), gives us

\[
\langle n|W(q, r)|n'\rangle = N_{nl}N_{n'l'} \sum_{kk'} \frac{(-1)^{k+k'}}{k!k'!} b^{-\xi} \left(\frac{n+l+\frac{1}{2}}{n-k}\right) \left(\frac{n'+l'+\frac{1}{2}}{n'-k'}\right) \int_0^\infty dr \, r^{d+\nu+2} e^{-\frac{(r^2+w)}{2}} j_\rho(sqr)
\]

At this point, the utility of Equation (E16) derived in Appendix E becomes very clear! We simply make the notational identifications as follows

\[
\xi \equiv l + l' + 2k + 2k' \quad \text{(4.56)}
\]
\[
d \equiv \xi + 2 + u \implies \kappa = \frac{\xi - \rho + u}{2} \in \mathbb{N}_0
\]
\[
\nu \equiv \frac{1}{b^2} + w \implies z = \frac{s^2 q^2}{4(1 + \frac{w^2}{4})}
\]

Rewriting Equation (4.55) with these identification yields

\[
\langle n|W(q, r)|n'\rangle = N_{nl}N_{n'l'} \sum_{kk'} \frac{(-1)^{k+k'}}{k!k'!} b^{-\xi} \left(\frac{n+l+\frac{1}{2}}{n-k}\right) \left(\frac{n'+l'+\frac{1}{2}}{n'-k'}\right) \int_0^\infty dr \, r^d e^{-\nu r^2} j_\rho(sqr)
\]

Applying Equation (E16) to the equation above, and staying consistent with the identifications in Equation (4.56) and (4.57), gives us

\[
\langle n|W(q, r)|n'\rangle = N_{nl}N_{n'l'} \sum_{kk'} \frac{(-1)^{k+k'}}{k!k'!} b^{-\xi} \left(\frac{n+l+\frac{1}{2}}{n-k}\right) \left(\frac{n'+l'+\frac{1}{2}}{n'-k'}\right) \int_0^\infty dr \, r^d e^{-\nu r^2} j_\rho(sqr)
\]

Applying Equation (E16) to the equation above, and staying consistent with the identifications in Equation (4.56) and (4.57), gives us

\[
\langle n|W(q, r)|n'\rangle = N_{nl}N_{n'l'} \sum_{kk'} \frac{(-1)^{k+k'}}{k!k'!} b^{-\xi} \left(\frac{n+l+\frac{1}{2}}{n-k}\right) \left(\frac{n'+l'+\frac{1}{2}}{n'-k'}\right) \int_0^\infty dr \, r^d e^{-\nu r^2} j_\rho(sqr)
\]

We would like to make Equation (4.58) more explicit, but also simplify it down, so that it doesn’t become too cumbersome. First, we notice that

\[
\left(\frac{1}{b^2} + w\right)^{-\frac{d-1}{2}} = b^{\xi + 3 + u} (1 + wb^2)^{-\frac{1}{2}(\xi + 3 + u)} = b^{\xi + 3 + u} (1 + wb^2)^{-\kappa - \frac{3}{2} - \frac{d}{2}}
\]
and, by manipulating the normalization factors from Equation (2.5), we get
\[
\sqrt{\frac{\pi}{4}} N_{nl} N_{n'l'} = b^{-3} \cdot \frac{1}{2^\rho} \frac{\pi n! n'!}{\Gamma(n + l + \frac{3}{2}) \Gamma(n' + l' + \frac{3}{2})} \tag{4.61}
\]

Overall, putting Equations (4.59) to (4.61) into (4.58) yields
\[
\langle n_r l_r | r^u e^{-wr^2} j_\rho(sqr) | n_{r'} l_{r'} \rangle = \frac{1}{2^{\rho+1}} \frac{\pi n_r! n_r'!}{\Gamma(n_r + l_r + \frac{3}{2}) \Gamma(n_{r'} + l_{r'} + \frac{3}{2})} b^u (sqr)^\rho e^{-z}
\]
\[
\times \sum_{k=0}^{n_r} \sum_{k'=0}^{n_{r'}} \left[ \frac{(-1)^{k+k'}}{k! k'!} \left( \frac{n_r + l_r + \frac{1}{2}}{n_r - k} \right) \left( \frac{n_r + l_r' + \frac{1}{2}}{n_r' - k'} \right) \right]
\times (1 + wb^2)^{-\kappa - \rho - \frac{3}{2}} \kappa! L_\kappa^{0+\frac{1}{2}}(z)
\]

where, \( \kappa = \frac{1}{2} (l_r + l_r' - \rho + u) + k + k' \in \mathbb{N}_0 \) and, \( z = \frac{(sqr)^2}{4(1 + wb^2)} \)

where we’ve restored the \( r \) for “relative,” and we remind the reader that the Gamma functions are defined as in Equation (F1), the generalized binomial coefficients are defined as in (F2), and the \( b \) is the harmonic oscillator length as defined in Equation (2.4).

In order to satisfy the condition that \( \kappa \in \mathbb{N}_0 \) in Equation (4.62), we’ll require that
\[
l_r + l_r' - \rho \in 2\mathbb{N}_0 \quad \text{and} \quad u \in 2\mathbb{N}_0 \tag{4.63}
\]
where we’ve imposed the latter restriction, \( u \in 2\mathbb{N}_0 \), by choice. The LHS restriction in Equation (4.63) is satisfied for us, since \( \rho \) represents the spherical harmonic rank of the two-body operator. In general, an operator can only change angular momentum in steps of its rank, by construction.* Finally, let’s reduce Equation (4.62) down to find the solution for Equation (4.51), by setting \( u = 0 = w \) and \( s = \sqrt{2} \), giving
\[
\langle n_r l_r | j_\rho(\sqrt{2}qr) | n_{r'} l_{r'} \rangle = \frac{1}{2^{\rho+1}} \frac{\pi n_r! n_r'!}{\Gamma(n_r + l_r + \frac{3}{2}) \Gamma(n_{r'} + l_{r'} + \frac{3}{2})} (\sqrt{2}qr)^\rho \exp \left( -\frac{q^2b^2}{2} \right)
\]
\[
\times \sum_{k=0}^{n_r} \sum_{k'=0}^{n_{r'}} \left[ \frac{(-1)^{k+k'}}{k! k'!} \left( \frac{n_r + l_r + \frac{1}{2}}{n_r - k} \right) \left( \frac{n_r + l_r' + \frac{1}{2}}{n_r' - k'} \right) \right]
\times \left[ \frac{1}{2} (l_r + l_r' - \rho) + k + k' \right]! L_\kappa^{0+\frac{1}{2}}(\frac{q^2b^2}{2})
\]

*this can be seen clearly when considering Equation (B14), for instance
4.5. Relative Bessel's Matrix Elements

4.5.1 RBMEs with Short-Range Correlations

In the case of neutrinoless double-beta decay, one could speculate that the exchange of the neutrino at high momenta (short range)\(^*\) would dominate. This would require the two neutrons involved in the \(0\nu\beta\beta\) decay to be probabilistically “closer” together, such that their relative wave-functions would overlap at the scale of roughly 3 fm \([120]\). This phenomenon is known as “short-range correlations” (SRCs), and can be physically modelled using the original prescription of Miller and Spencer \([121]\). The importance of SRCs for \(0\nu\beta\beta\) NMEs was recognized by \([116, 122]\), and further popularized by \([123]\). Now many modern calculations include several parameterizations of SRCs for neutrinoless double-beta decay \([71, 72, 115, 117, 118, 124–134]\).

To implement SRCs, one simply updates the nucleon-nucleon radial wave-function as

\[
R_{nl}(r) \rightarrow [1 + J(r_{12})]R_{nl}(r)
\]

(4.65)

where the function, \(J(r_{12})\), is fit as a “Jastrow-type” function, such that

\[
J(r_{12}) = -ce^{-ar_{12}^2}(1 - br_{12}^2)
\]

(4.66)

The numbers \(a, b, c \in \mathbb{R}\) are called “SRC parameters,” and many physics-dependant fittings have been made for them \([121]\). Notice that the correct variable to use for the Jastrow-type function in Equation (4.65) is \(r_{12}\), as in (4.29), since that is the coordinate space in which the SRC parameters have been fit. The most commonly used sets of SRC parameters for \(0\nu\beta\beta\) are given in Table 4.1 below.

<table>
<thead>
<tr>
<th>Name</th>
<th>Abbr.</th>
<th>(a \text{ [fm}^{-2})</th>
<th>(b \text{ [fm}^{-2})</th>
<th>(c) [1]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Argonne V18 Potential</td>
<td>AV18</td>
<td>1.59</td>
<td>1.45</td>
<td>0.92</td>
</tr>
<tr>
<td>Charge-Dependant Bonn Potential</td>
<td>CD-Bonn</td>
<td>1.52</td>
<td>1.88</td>
<td>0.46</td>
</tr>
<tr>
<td>Miller-Spencer Fitting</td>
<td>MS</td>
<td>1.1</td>
<td>0.68</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 4.1: Common SRC parameters for the Jastrow-type function in Equation (4.66), to be used in (4.65) for neutrinoless double-beta decay.

To implement SRCs in our \(M^{0\nu}\) TBMEs, we apply the mapping in Equation (4.65) with (4.66) on the RBMEs as in Equation (4.51). That is

\[
\langle n_r | j_\rho(q \cdot r_{12}) | n'_l \rangle \rightarrow \int_0^\infty dr \, r^2 [1 - ce^{-as^2r^2}(1 - br^2)]^2 R_{n_r l}(r) \langle n_r | j_\rho(q \cdot r_{12}) R_{n_l l'}(r) \rangle
\]

(4.67)

It is easy to show that, for some \(s \in \mathbb{R}\),

\[
[1 - ce^{-as^2r^2}(1 - bs^2r^2)]^2 = 1 - 2be^{-as^2r^2} + 2bc^2s^2r^2 e^{-as^2r^2} + c^2 e^{-2as^2r^2} - 2bc^2s^2r^2 e^{-2as^2r^2} + b^2c^2s^4r^4 e^{-2as^2r^2}
\]

(4.68)

At this point, the utility of Equation (4.62) becomes clear. Let’s make the labelling

\[
T_{n_r, l_r, n'_l, l'_r}^{u, u; s} (q) \equiv \langle n_r | l_r | r^u e^{-wr} j_\rho(sqr) | n'_l l'_r \rangle
\]

(4.69)

\(^*\)relative to inter-nucleonic momenta
4.6 Reconstructing $M^{0\nu}$ TBMEs

so, plugging Equation (4.68) into (4.67), and using the notation in (4.69), gives

\[
\langle n_r l_r | j_\rho (\sqrt{2} q r) | n'_r l'_r \rangle \rightarrow \mathcal{T}^{0,0;\sqrt{2}}_{n_r l_r, n'_r l'_r}(q) - 2c \mathcal{T}^{0,2a;\sqrt{2}}_{n_r l_r, n'_r l'_r}(q) + 4bc \mathcal{T}^{2,2a;\sqrt{2}}_{n_r l_r, n'_r l'_r}(q) + 2c^2 \mathcal{T}^{4,2a;\sqrt{2}}_{n_r l_r, n'_r l'_r}(q)
\]

(4.70)

Using Equation (4.70) along with (4.62) will incorporate SRCs into our TBMEs from Equations (4.31), (4.46), and (4.50). It should be noted that the $b$ in Equation (4.70) above is an SRC parameter from (4.66), whereas the $b$ in Equation (4.62) is the harmonic oscillator length from (2.4). Thus, it is necessary to distinguish $b \rightarrow b_{osc}$, or alike, when computing Equation (4.62), to avoid ambiguity.

4.6 Reconstructing $M^{0\nu}$ TBMEs

Since we have introduced lots of new notation in this chapter, for the reader's convenience we will summarize the formulas derived above. To obtain the $0\nu\beta\beta$ NMEs

\[
M^{0\nu} = M_{GT}^{0\nu} - \left( \frac{g_N}{g_A} \right)^2 M_{F}^{0\nu} + M_{T}^{0\nu}
\]

(3.21)

where,

\[
M^{0\nu}_\alpha = \langle f | \hat{M}^{0\nu}_\alpha | i \rangle, \quad \alpha = GT, F, T
\]

(3.22)

we use Equation (4.1) in combination with the TBMEs

\[
M^{0\nu}_{abcd} \equiv \langle a b : J || \hat{M}^{0\nu}_\alpha || c d : J' \rangle, \quad \alpha = GT, F, T
\]

(4.2)

In general, using the closure approximation via Assumption 2, we can write

\[
M^{0\nu}_{abcd} = \delta_{ac, bd} \frac{2R}{\pi} \int_0^\infty dq \frac{q \cdot h_\alpha(q^2)}{q + E^{cl}_0} \langle a b : J || \hat{Q}_\alpha || c d : J' \rangle
\]

(4.71)

where the form factors, $h_\alpha$, are

\[
h_F(q^2) \equiv \frac{g_F^2(q^2)}{g_{V,0}^2}
\]

(4.11)

\[
h_{GT}(q^2) \equiv \frac{1}{g_{A,0}^2} \left[ g_A^2(q^2) - \frac{g_A(q^2) g_V(q^2) q^2}{3m_p} + \frac{g_P^2(q^2) q^4}{12m_p^2} + \frac{g_M^2(q^2) q^2}{6m_p^4} \right]
\]

\[= \frac{g_A^2(q^2)}{g_{A,0}^2} \left[ 1 - \frac{2}{3} \frac{q^2}{q^2 + m^2} + \frac{1}{3} \left( \frac{q^2}{q^2 + m^2} \right)^2 \right] + \frac{1}{6} \frac{g_M^2(q^2) q^2}{g_{A,0}^2 m_p^2}
\]

(4.12)
with the $g$-factors

$$g_Y(q^2) \equiv \frac{g_{Y,0}}{(1 + q^2/L_Y^2)^2}, \quad g_A(q^2) \equiv \frac{g_{A,0}}{(1 + q^2/L_A^2)^2}$$

$$g_P(q^2) \equiv \frac{2m_p g_A(q^2)}{q^2 + m_n^2}, \quad g_M(q^2) \equiv \left(\frac{\mu_p - \mu_n}{\mu_N}\right) g_Y(q^2)$$ (4.14)

The augmented operators, $\tilde{Q}_\alpha$ (which are $q$-dependent), have been defined respectively in Equations (4.33), (4.49), and (4.19), which can be written collectively as

$$\tilde{Q}_\alpha \equiv \begin{cases} \sqrt{4\pi} j_0(q \cdot r_12) \tilde{Y}_0 \sigma_1 \sigma_2, & \alpha = \text{GT} \\ \sqrt{4\pi} j_0(q \cdot r_12) \tilde{Y}_0 \mathbb{1}, & \alpha = \text{F} \\ \sqrt{2\pi} j_2(q \cdot r_12) \tilde{Y}_2 \tilde{S}_{12}, & \alpha = \text{T} \end{cases}$$ (4.72)

The TBMEs for the GT and F augmented operators are as follows:

$$\langle ab : J || \tilde{Q}_\text{GT} || cd : J' \rangle = \delta_{J,J'} \sum_{S=0,1} \sigma \sigma(S) \left[ \sum_L \left[ \begin{array}{ccc} l_a & l_b & L \\ \frac{1}{2} & \frac{1}{2} & S \\
_l & j_b & J \end{array} \right] \left[ \begin{array}{ccc} l_c & l_d & L \\ \frac{1}{2} & \frac{1}{2} & S \\
_c & j_d & J \end{array} \right] \right] \sum_{n_r l_r, n_r' l_r'} D_{cd}^{n_r, n_r'} \langle n_r l_r | j_0(\sqrt{2qr}) | n_r' l_r' \rangle$$

with the spin eigenvalues

$$\sigma \sigma(S) \equiv 2S(S + 1) - 3 = \left\{ \begin{array}{cl} 1, & S = 1 \\ -3, & S = 0 \end{array} \right.$$ (4.40)

and

$$\langle ab : J || \tilde{Q}_\text{F} || cd : J' \rangle = \delta_{J,J'} \sum_{L,S} \left[ \begin{array}{ccc} l_a & l_b & L \\ \frac{1}{2} & \frac{1}{2} & S \\
_l & j_b & J \end{array} \right] \left[ \begin{array}{ccc} l_c & l_d & L \\ \frac{1}{2} & \frac{1}{2} & S \\
_c & j_d & J \end{array} \right] \sum_{n_r l_r, n_r' l_r'} D_{ab} D_{cd}^{n_r, n_r'} \langle n_r l_r | j_0(\sqrt{2qr}) | n_r' l_r' \rangle$$

(4.50)

with the sums over $S = 0, 1$ and $\Delta(l_a l_b : L)$, and the Talmi-Moshinsky brackets are

$$D_{ab} = \langle n_r l_r, N\Lambda : L | n_a l_a, n_b l_b : L \rangle \quad \text{and} \quad D_{cd}^{n_r', n_r'} = \langle n_r' l_r, N\Lambda : L | n_c l_c, n_d l_d : L \rangle$$ (4.44)

with the CTML adapted from Equation (D16) as
4.6. Reconstructing $M^{\alpha\nu}$ TBMES

\[
\sum_{n_r l_r., n_r' l_r'} = \left\{ \begin{array}{c}
[(\epsilon_{ab}+L)/2]-(n_r+N) & [(\epsilon_{ab}-L)/2]-n_r & [(\epsilon_{ab}-L)/2] \\
\sum
(6) l_r = [(\epsilon_{ab}-L)/2]-(n_r+N) & \sum
(5) N = 0 & \sum
(3) n_r = 0
\end{array} \right.
\]

(4.73)

where the bolded, parenthesized, left superscripts denote the order that each parameter in the limits should be set. The TBMES for the T augmented operator is as follows:

\[
\langle ab; J||\hat{Q}_T||cd; J'\rangle = \delta_{J,J'} \sum_{LL'} 2\sqrt{5} (1)^{1+L+L'} \hat{L} \hat{L}' \left\{ \begin{array}{c}
L & 1 & J \\
L' & 2 
\end{array} \right\}
\]

\[
\times \left[ \begin{array}{ccc}
l_a & l_b & L \\
\frac{1}{2} & \frac{1}{2} & 1
\end{array} \right] \left[ \begin{array}{ccc}
l_c & l_d & L' \\
\frac{1}{2} & \frac{1}{2} & 1
\end{array} \right] \left[ \begin{array}{ccc}
j_a & j_b & J \\
j_c & j_d & J
\end{array} \right]
\]

\[
\times \sum_{n_r l_r., n_r' l_r'} D_{ab} D_c^{d'} (1)^{L'+l_r+\Lambda} \left\{ \begin{array}{ccc}
L & l_r & \Lambda \\
l_r' & L' & 2
\end{array} \right\}
\]

\[
\times \sqrt{6} (l_r 0 2 0 | l_r' 0) \hat{L}_r \langle n_r l_r; j_2 (\sqrt{2}qr) | n_r' l_r' \rangle
\]

with the sums over $\Delta(l_a l_b; L)$ and $\Delta(l_c l_d; L')$, and the Talmi-Moshinsky brackets

\[
D_{ab} = \langle n_r l_r, NA; L | n_a l_a, n_b l_b; L \rangle \quad \text{and} \quad D_c^{d'} = \langle n_r' l_r', NA; L' | n_c l_c, n_d l_d; L' \rangle
\]

(4.28)

with the CTML adapted from Equation (D21) as

\[
\sum_{n_r l_r., n_r' l_r'} = \left\{ \begin{array}{c}
[(\epsilon_{ab}+L)/2]-(n_r+N) & [(\epsilon_{ab}-L)/2]-n_r & [(\epsilon_{ab}-L)/2] \\
\sum
(8) l_r' = [\Lambda-L'] & \sum
(6) l_r = [(\epsilon_{ab}-L)/2]-(n_r+N) & \sum
(5) N = 0 & \sum
(4) n_r = 0
\end{array} \right.
\]

(4.74)

with the constraints: (9) $\Delta(l_r, l_r'; 2)$, (3) $\Delta(LL'; 2)$, (2) $\Delta(l_c l_d; L')$, (1) $\Delta(l_a l_b; L)$,

\[
\epsilon_{ab} = 2n_a + l_a + 2n_b + l_b, \quad \epsilon_{cd} = 2n_c + l_c + 2n_d + l_d
\]

(4.75)

To analytically calculate the RBMES, we may use

\[
\langle n_r l_r | j_\rho (\sqrt{2}qr) | n_r' l_r' \rangle = \frac{1}{2^{n_r+1}} \sqrt{\frac{\pi n_r! n_r'!}{\Gamma(n_r + l_r + \frac{3}{2}) \Gamma(n_r' + l_r' + \frac{3}{2})}} (\sqrt{2}q b) \exp \left( -\frac{q^2 b^2}{2} \right)
\]

\[
\times \sum_{k=0}^{n_r} \sum_{k'=0}^{n_r'} \left[ \frac{(\rho+1)^{n_r + l_r + \frac{1}{2}}}{k! k'} \left( \begin{array}{c}
n_r + l_r + \frac{1}{2} \\
n_r - k
\end{array} \right) \left( \begin{array}{c}
n_r' + l_r' + \frac{1}{2} \\
n_r' - k'
\end{array} \right) \right]
\]

(4.64)

or, to incorporate SRCs, use

\[
\langle n_r l_r | j_\rho (\sqrt{2}qr) | n_r' l_r' \rangle \rightarrow \mathcal{I}_{n_r l_r n_r' l_r'}^{0,0; \sqrt{2}} (q) - 2c \mathcal{I}_{n_r l_r n_r' l_r'}^{0, 2a; \sqrt{2}} (q) + 4bc \mathcal{I}_{n_r l_r n_r' l_r'}^{2, 2a; \sqrt{2}} (q)
\]

(4.70)
4.6. Reconstructing $M^{0\nu}$ TBMEs

with

$$\mathcal{I}_{n_r l_r, n'_r l'_r}^{u,w,s}(q) = \frac{1}{2^{\rho+1}} \sqrt{\frac{\pi n_r! n'_r!}{\Gamma(n_r + l_r + \frac{1}{2}) \Gamma(n'_r + l'_r + \frac{1}{2})}} b^u (sqb)^{\rho} e^{-z} \times \sum_{k=0}^{n_r} \sum_{k'=0}^{n'_r} \left[ (-1)^{k+k'} \frac{k! k'!}{(n_r + l_r + \frac{1}{2}) \binom{n_r + l_r + \frac{1}{2}}{n_r - k} \binom{n'_r + l'_r + \frac{1}{2}}{n'_r - k'}} \times (1 + w b^2)^{-\kappa - \frac{3}{2} \rho} \kappa! \frac{L_\kappa^{\rho + \frac{1}{2}}(z)}{4(1 + w b^2)} \right]$$

(4.62)

where, $\kappa = \frac{1}{2} (l_r + l'_r - \rho + u) + k + k' \in \mathbb{N}_0$ and, $z = \frac{(sqb)^2}{4(1 + w b^2)}$

where the $b$ in this formula represents the oscillator length,* and

$$\mathcal{I}_{n_r l_r, n'_r l'_r}^{u,w,s}(q) \equiv \langle n_r l_r | r^u e^{-wr^2} j_\rho(sqr) | n'_r l'_r \rangle$$

The formulae above constitute the most mathematically laborious component of this research, and unfortunately that carries into their numerical treatment. Controlling the necessary integrations and computationally heavy summations involved, in both a precise and efficient manner, is not a trivial matter. More on this will be discussed in Section 6.4. Once we’ve dealt with the numerical issues, there is one last step that we should not forget! In order to capture the fermionic statistics of our nucleons, we will need to anti-symmetrize the TBMEs using Theorem B.4.

\[ \langle a b; J || \hat{M}_{\alpha}^{0\nu} || c d; J' \rangle \longrightarrow \langle a b; J || \hat{M}_{\alpha}^{0\nu} || c d; J' \rangle \]

Now that the $0\nu\beta\beta$ operators are mathematically in order, we’d like to find a way to embed this physics into nuclear structure. We’ll accomplish this task by using the nuclear many-body method known as: the valence space in-medium similarity renormalization group.

*not to be confused with the $b$ from the SRC parameters!
Chapter 5

Valence Space In-Medium Similarity Renormalization Group

As introduced in Section 2.2, the ultimate goal of nuclear physics is to fully solve the nuclear Schrödinger equation. With this dynamics in place, all the properties of the nucleus, as a semi-classical quantum mechanical object, can be modelled completely. The two major issues are: how do we obtain an appropriate potential that describes low-energy QCD, and how can we numerically handle such a large Hamiltonian? Making both of these problems computationally tractable is where $\chi$EFT and nuclear many-body methods come into play.

The non-perturbative, ab initio approach that we will use is known as the “Valence Space In-Medium Similarity Renormalization Group” (VS-IM-SRG) method [135]. There are currently several versions of IM-SRG [136], but we’ll choose the Magnus Formulation, as outlined in Section 5.4. In terms of the acronym, the VS-IM-SRG will be summarized in the order:* Valence Space (VS), Similarity Renormalization Group (SRG), and then In-Medium (IM).

5.1 Nuclear Core and Valence Space

As with most nuclear many-body methods, we’ll start by modelling the nucleus using the ShM. However, as nuclei become large in mass number, the number of interactions and potential excitation configurations between protons and neutrons in their shells increases dramatically. How can we contain the nucleus in such a way that is computationally manageable? Referring back to Figure 2.1, one could imagine that there exists a Fermi energy that limits the dynamics of nucleons lying in lower closed shells. We’ll take advantage of this, and define what is known as a “nuclear core”† of nucleons which we force to be inert under renormalization.

Assumption 3

Nuclei with a large enough $Z$ and $N$ can be modelled statistically using a Fermi surface to define an inert nuclear core, within the context of the ShM. We’ll assume that this approximation is good at reproducing reality.

*This order somewhat reflects how VS-IM-SRG was developed chronologically
†Such a core should not be confused with the antiquated idea of a “hard core” as defined by the nuclear potential, which we discuss more in Section 5.2.1 below.
5.1. Nuclear Core and Valence Space

Figure 5.1: Core, valence space, and excluded region for the ground state of $^{48}$Ca within the nuclear shell model. The orange arrows represent undesirable, low-probability excitations past the Fermi surface or into the excluded region, and the green arrows represent excitations allowed within the defined valence space. The purple arrow schematically represents the use of VS-IM-SRG to renormalize the dynamics to the chosen valence space, in this case the $pf$-shell (which rarely includes the $0g_{9/2}$ orbit, despite its small energy gap to $1p_{1/2}$ relative to the $0f_{7/2}$ and $1p_{3/2}$ gap), thus leaving the core inert and the excluded region empty. Since $^{48}$Ca is doubly magic, this valence space accepts no protons, which makes $^{48}$Ca a favourable nucleus as a theoretical benchmark.

Once a core has been established, this leaves a indefinite region of infinitely many shells that nucleons may excite into. Yet, it’s clear that excitations from the ground state to higher lying orbits are less probable than excitations into lower lying orbits. Thus, we find it reasonable to excise higher lying shells from the nucleonic dynamics, in a space called the “excluded region.” What is left is known as the “valence space” (VS), since this is where the dynamics of the valence nucleons* can occur. We see that an a priori choice of valence space automatically defines the core and excluded regions, as depicted for Calcium-48 in Figure 5.1.

Assumption 4
Coupled with Assumption 3 above, a suitable choice of valence space, tailored to a particular nucleus, should be able to capture enough dynamics in order to reproduce said nuclei’s properties. Of course, this inherently depends on the efficacy of the nuclear many-body method.

5.1.1 Model Space
To build the nuclear ShM, we’ll start with the oscillator† basis (see Section 2.1.1) for the single-particle wave-functions. To construct the nuclear wave-function we’ll use a Slater determinant‡

---

* those which lie above the Fermi surface defining the inert core
† including all the accepted corrections needed to reproduce the observed magic numbers
‡ our single-particles are nucleons, which are fermions, and hence a Slater determinant is justified
5.2. Similarity Renormalization Group

(see Section 2.1.3). However, as opposed to the standard ShM, we’ll now want to decouple these wave-functions into the core and valence space respectively, as mentioned above. Therefore, within the valence space, we need to specify how many single-particle excitations will be acceptable for our calculations. This is done by setting a model space “size” known either as “$N_{\text{max}}$” or “$e_{\text{max}}$” for all single-particle states, in accordance with Equation (2.2), like

$$2n + l \leq e_{\text{max}}$$

Upon the inclusion of a 3N interaction, it would then also be important to set an “$E_{3\text{max}}$” like

$$e_{\text{max}}^{(1)} + e_{\text{max}}^{(2)} + e_{\text{max}}^{(3)} \leq E_{3\text{max}}$$

where the parenthesized superscripts label some set of three separate single-particles in the valence space Slater determinant. We will exclusively set $E_{3\text{max}} = 14$ for our calculations, but vary $e_{\text{max}}$ due to the following physically intuitive remark:

**Remark 5.1**

Upon applying the nuclear ShM for a valence space nuclear many-body method, as the size of the model space ($e_{\text{max}}, E_{3\text{max}}, \ldots$) increases, the results will become independent of the oscillator frequency ($\hbar \omega$) used for the basis states, resulting in “converge” [137].

5.2 Similarity Renormalization Group

Glasek and Wilson took the renormalization group, the use of which in physics had been pioneered in the early 1970’s by Wilson and alike [138], and modernized it in an ingenious way [139, 140]. In essence, the renormalization group is a tool to systematically view physical structure at different scales (distance, energy, etc) [141]. The idea was to apply the renormalization group in such a way that as an energy parameter decreases, the Hamiltonian diagonalizes in a self-consistent way. Exploiting this self-similarity of the Hamiltonian under the renormalization group is what gave this scheme the name “Similarity Renormalization Group” (SRG).

The similarity transformation of the Hamiltonian can be written as

$$\tilde{H} = U \hat{H} U^{-1} \quad (5.1)$$

where $U$ is the unitary (similarity) matrix, hence $U^{-1} = U^\dagger$. The motivation behind Equation (5.1) is that Wilson and Glasek wanted to find a way to remove the off-diagonal terms of the Hamiltonian, but in doing so, preserve the observables of the system of interest. For instance, we can calculate the spectrum normally or within the SRG space

$$E_n = \langle \Psi_n | \hat{H} | \Psi_n \rangle = \langle \Psi_n | U^\dagger (U \hat{H} U) U | \Psi_n \rangle = \langle \Psi_n | \tilde{H} | \Psi_n \rangle$$

The details behind how one drives the Hamiltonian to a band or block-diagonal form are outlined in Section 5.2.2 below. Clearly, a block-diagonal Hamiltonian is not only advantageous in the framework of QFT, since all that would be needed to find the eigenstates of any physical
system are a set of sub-block diagonalizations of the transformed Hamiltonian. The use of the renormalization group in nuclear physics, for instance, has been utilized in recent studies [6].

5.2.1 Nuclear Potentials and Similarity Transformations

QCD has the favourable quality that as the energy of interest increases, the theory becomes perturbatively renormalizable [44], due to the running of the strong coupling constant for the gluon, $\alpha_S$, as a function of the transfer momentum $^*$

$$\alpha_S(q^2) = \frac{\alpha_S(\mu^2)}{1 + B\alpha_S(\mu^2) \ln(q^2/\mu^2)}$$

This property is known as “asymptotic freedom,” which was discovered independently in 1973 by Gross and Wilczek [142] and Politzer [143]. The subsequent renormalizability and lack of Landau poles make quantum chromodynamics UV complete. Unfortunately, for the low-energy regime, $^+$ such as those found in nuclear physics, the coupling constant is of order unity, yielding an infrared divergence. Ergo, the standard perturbative techniques used in QFT commonly fail within the context of nuclear theory.

Since the Dirac equation governs physics at high energies, and the Schrödinger equation governs quantum mechanics at low energies, we can consider the nuclear problem as an exercise in solving the nuclear Schrödinger Hamiltonian. With this perspective, where do these perturbative divergences manifest? The off-diagonal terms of the Hamiltonian physically represent the correlation between high and low momentum states. Since the nuclear Hamiltonian is so large, one may propose to use SRG technology, as in Equation (5.1), to “soften” the nuclear interactions and drive the off-diagonal terms to zero [8]. A useful visualization of this can be seen in Figures 9 and 10 on page 102 of [8]. $^\‡$

This softening is an intuitive suggestion, since the renormalization group is what determines: the running of LECs, power counting methodology, and regularization cutoff analysis in $\chi$EFT interactions (see Section 2.2.3). It therefore makes sense to adopt SRG technology for nuclear potentials in an ab initio model. However, with this SRG framework we must let go of the classical notion in nuclear physics that there exists a repulsive “hard core.” $^\§$ Why? Many SRG evolved potentials might not display this hard core, but they still describe the exact same observables as the bare potential. It is easy to argue that this is an acceptable theoretical compromise, since the potential is ultimately not an observable itself, hence it cannot be measured, and it should not be interpreted physically [8]. Furthermore, these studies have motivated the recently discovered fact that many-body interactions, like 3N forces, are important for nuclear

---

$^*$ $B > 0$ for a QFT with three colours and six quarks, and $q^2 = \mu^2$ is a mass scale where one can confidently measure the colour charge of a quark.

$^+$ at around roughly the mass of the proton, 1 GeV, and subsequent hadronization scales

$^\‡$ More diagrams, specifically in the context of IM-SRG, can been seen in Figure 26 of [28] or Figure 10.2 of [144] for a numerical example, among others.

$^\§$ Note that the idea of this nucleon-nucleon repulsive “core” is very different from the nuclear core as depicted in Figure 5.1.
physics [145]. How one might capture these interactions will be touched on in Section 5.3. But first, if we make the SRG a necessary step for our nuclear many-body method - how does one mathematically accomplish the desired decouplings?

### 5.2.2 SRG Flow Equations

We begin with the similarity transformation from Equation (5.1), but parameterize it by a “flow parameter,” \( s \in \mathbb{R} \), as [140] originally introduced.* As we increase this flow parameter, we’ll evolve the Hamiltonian in infinitesimal regulations through the resolution scales of the renormalization group, in order to drive \( \hat{H} \) towards a block-diagonal form. This can be accomplished by first requiring that

\[
\hat{H}_s = U_s \hat{H} U_s^\dagger = \hat{T}_{\text{rel}} + V_s
\]

where, \( \hat{H} = \hat{T}_{\text{rel}} + V \)

That is; the relative kinetic energy term remains unchanged under the similarity transformation. For a valence space formulation of the SRG, we decouple the valence space (VS) and excluded region (excl), and write the similarity transformation as

\[
\hat{H}_s = U_s \hat{H} U_s^\dagger = \hat{H}_s^{\text{VS}} + \hat{H}_s^{\text{excl}}
\]

and then we obtain the eigenstates by a diagonalization within the valence space [137].

In order to solve for \( \hat{H}_s \), one can construct an ODE for it by taking the derivative of Equation (5.2) with respect to \( s \):

\[
\frac{d}{ds} \hat{H}_s = \frac{d}{ds} U_s \hat{H} U_s^\dagger + U_s \frac{d}{ds} \hat{H} U_s^\dagger = \frac{d}{ds} (U_s^\dagger \hat{H}_s U_s) U_s^\dagger + U_s (U_s^\dagger \hat{H}_s U_s) \frac{d}{ds} U_s^\dagger
\]

\[
= \frac{d}{ds} U_s^\dagger \hat{H}_s + \hat{H}_s U_s \frac{d}{ds} U_s^\dagger
\]

(5.3)

noting that \( d\hat{H}/ds = 0 \), since it is an initial condition; and that \( U_s U_s^\dagger = 1 \), since \( U_s \) is unitary. By intuition, we’d like to isolate the derivative of \( U_s^\dagger \) in terms of the derivative of \( U_s \), which we can do by (once again) appealing to unitarity

\[
\frac{d}{ds} (U_s^\dagger U_s) = \frac{d}{ds} 1 = 0 \implies \frac{d}{ds} U_s^\dagger U_s = -U_s^\dagger \frac{d}{ds} U_s
\]

\[
\frac{d}{ds} U_s^\dagger = -U_s^\dagger \frac{d}{ds} U_s
\]

(5.4)

Plugging Equation (5.4) into (5.3) yields

---

*They labelled the flow parameter \( \lambda \), since it was thought of as a regularization cutoff, and they had already labelled the unitary matrix performing the similarity transformation as \( S \), instead of \( U \).
5.2. Similarity Renormalization Group

\[
\frac{d\tilde{H}_s}{ds} = \frac{dU_s^*}{ds} U_s^* \tilde{H}_s - \tilde{H}_s \frac{dU_s}{ds} U_s^* \tag{5.5}
\]

And so, by making the definition

\[
\eta_s \equiv \frac{dU_s}{ds} U_s^* \tag{5.6}
\]

we may rewrite Equation (5.5) in the compact form

\[
\frac{d\tilde{H}_s}{ds} = [\eta_s, \tilde{H}_s] \tag{5.7}
\]

Equation (5.7) is referred to as the “flow equation,” and \(\eta_s\) is called the “generator” of this flow, of which many choices can be found \([146, 147]\). Notice that taking the dagger of Equation (5.6) shows that \(\eta_s\) is anti-hermitian

\[
\eta_s^\dagger = \left( \frac{dU_s}{ds} U_s^* \right)^\dagger = U_s \frac{dU_s^\dagger}{ds} = -\frac{dU_s}{ds} U_s^* = -\eta_s
\]

where the equivalence, denoted by \(\overset{\approx}{=}\), comes from Equation \(U_s \times (5.4)\). \(\eta_s\) being anti-hermitian justifies referring to it as a generator, since we can mathematically identify \(U_s\) by solving

\[
\frac{dU_s}{ds} = \eta_s U_s \implies U_s(\Lambda) = S \exp \left[ \int_{\Lambda}^{s} ds' \eta_s' \right] \tag{5.8}
\]

where \(S\) is the \(s\)-ordering operator, such that it reorders operators from left to right in descending \(s'\); and \(\Lambda\) is some arbitrarily small cutoff, which yields self-similarity of the Hamiltonian, i.e., \(\lim_{s \to \Lambda} \tilde{H}_s = \tilde{H}\). Physically, Equation (5.8) can be read as \(\eta_s\) infinitesimally generating changes to the resolution scale encoded by the similarity transformation in (5.2), which justifies calling \(s\) a flow parameter. Notice that had we been interested in reproducing the high-energy physics of QCD, one could imagine simply reversing the \(s\)-ordering operator, flip the integral, and set \(\Lambda\) to be arbitrarily large.

For our purposes, we will take \(\Lambda = 0\), and require that the unitary matrix, \(U_s\), be constructed such that the Hamiltonian is block-diagonal as the flow increases. That is, splitting\(^*\) the similarity transformed Hamiltonian into “diagonal” (d) and “off-diagonal” (od) terms

\[
\tilde{H}_s = \tilde{H}_s^d + \tilde{H}_s^{od} \tag{5.9}
\]

we want a generator that guarantees

\[
\lim_{s \to \infty} \tilde{H}_s^{od} = 0
\]

Not all generators yield the desired block diagonal form, and different choices of generators is still an ongoing avenue of research \([136]\).

\(^*\)The decomposition of operators in this manner is somewhat roughly defined, in terms of what deems “band” or “block” diagonal, and depends on the intended purpose of the SRG.
5.2. Similarity Renormalization Group

Choice of Generator

Since the genesis of the SRG flow equations, several generators have been suggested which evolve the Hamiltonian to a block diagonal form. One of the earliest choices of $\eta_s$ with practical use is the Wegner generator [146], take as

$$\eta_s \equiv [\tilde{H}^d_s, \tilde{H}^{od}_s] + \text{h.c.}$$

It can be shown that the Wegner generator, under its use with Equation (5.7), will give the desired asymptotics for the off-diagonal entries of the Hamiltonian

$$\tilde{H}_{ij}(s) \sim e^{-s\Delta^2_{ij}} \tilde{H}_{ij}(0) \quad \text{where,} \quad \Delta_{ij} \equiv \tilde{H}^d_{ii}(s) - \tilde{H}^d_{jj}(s)$$

Shortly thereafter, in an application of quantum many-body theory to chemistry, White proposed a new generator of the form [147]

$$\eta_{ij}(s) = \tilde{H}^{od}_{ij}(s) / \Delta_{ij} + \text{h.c.} \quad (5.10)$$

which has the asymptotics

$$\tilde{H}_{ij}(s) \sim e^{-s\tilde{H}_{ij}(0)}$$

The White generator has a more controlled suppression of the off-diagonal terms than the Wegner generator. Hence, despite potential numerical instabilities with the energy denominator in Equation (5.10), unless otherwise stated we will opt to use the White generator.

5.2.3 Consistent Operator Evolution

Of course, the energy levels are not the only property of a nucleus we seek to understand, and hence the Hamiltonian is not the only operator that we wish to SRG evolve. For instance, one may wish to model: electromagnetic properties, radii, GT transitions, and double-beta decay. All these observables will be described by some Hermitian operator, which we’ll label generically as $\hat{O}$. One of the useful features about the SRG transformation is that the same evolution may be applied to $\hat{O}$ along with $\hat{H}$. That is, we can generalize Equation (5.2) to

$$\hat{O}_s = U_s \hat{O} U_s^\dagger \quad (5.11)$$

and use the same manipulations as above to arrive at the operator flow equation

$$\frac{d\hat{O}_s}{ds} = [\eta_s, \hat{O}_s] \quad (5.12)$$

Applying Equation (5.12) along with (5.7), in tandem, can only be performed consistently as long as the same generator is used. One should note that as we add more operators using this technique, we effectively must solve more ODEs - which highlights a computational limitation of this formulation. To over come this inefficiency, we’ll use the Magnus expansion with IM-SRG,
5.3 Reference State Normal Ordering

Applying the SRG flow equations to the nuclear Hamiltonian has typically been done in free space, to make 2N and 3N nucleonic interactions more manageable [148]. For our purposes, however, we need a way to translate $\tilde{H}_s$ into the language of our desired valence space, as outlined in Section 5.1. That is, we’d like to renormalize our $\chi$EFT interactions to match Figure 5.1. Remarkably, this can be accomplished by redefining normal ordering “In-Medium” (IM) - with respect to the nuclear core. Along with this, we can induce 3N effects into 2N terms, thus capturing many-body physics upon truncation for free.

As introduced in Section C.1, the necessity to normal order creation and annihilation operators is ingrained in the machinery of second quantization. In QFT, this is often done with respect to the vacuum, but can we generalize this notion? Instead of normal ordering against the vacuum, we can indeed normal order with respect to some reference state $|\Phi_0\rangle$. All that we need to do is impose a new definition of normal ordering in Equation (C10) via

$$\langle 0| \hat{c}_i^\dagger \cdots \hat{c}_j |0\rangle = 0 \quad \rightarrow \quad \langle \Phi_0| \hat{c}_i^\dagger \cdots \hat{c}_j |\Phi_0\rangle = 0$$

(5.13)

For a second quantized Hamiltonian,

$$\hat{H} = \sum_{ab} \hat{T}_{ab} \hat{c}_a^\dagger \hat{c}_b + \frac{1}{2!} \sum_{abcd} V_{abcd}^\langle (2N) \rangle \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_c \hat{c}_d + \frac{1}{3!} \sum_{abcdef} V_{abcdef}^\langle (3N) \rangle \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_c^\dagger \hat{c}_d \hat{c}_e \hat{c}_f + \cdots$$

(5.14)

we can then use Wick’s Theorem (see Equation (C12) of Section C.1.1) with the “reference state normal ordering” from Equation (5.13) to rewrite (5.14) as [136, 149]

$$\hat{H} = E + \sum_{ab} F_{ab} |\hat{c}_a^\dagger \hat{c}_b| + \frac{1}{2!} \sum_{abcd} U_{abcd} |\hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_c \hat{c}_d| + \frac{1}{3!} \sum_{abcdef} W_{abcdef} |\hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_c^\dagger \hat{c}_d \hat{c}_e \hat{c}_f|$$

(5.15)

where

$$E = \sum_a \hat{T}_{aa} n_a + \frac{1}{2} \sum_{ab} V_{abab}^\langle (2N) \rangle n_a n_b + \frac{1}{6} \sum_{abc} V_{abcabc}^\langle (3N) \rangle n_a n_b n_c$$

(5.16)

$$F_{ab} = \hat{T}_{ab} + \sum_c V_{abac}^\langle (2N) \rangle n_c + \frac{1}{2} \sum_{cd} V_{acdbcd}^\langle (3N) \rangle n_c n_d$$

(5.17)

$$U_{abcd} = V_{abcd}^\langle (2N) \rangle + \sum_e V_{abcde}^\langle (3N) \rangle n_e$$

(5.18)

$$W_{abcdef} = V_{abcdef}^\langle (3N) \rangle$$

(5.19)
with \( n_a \) and alike denoting the occupation numbers of nucleons in the reference state.

This is a powerful result! We see that even if we truncate the reference state normal ordered Hamiltonian in Equation (5.15) at the 2N level, we can still capture the bulk of the 3N interactions via Equations (5.16) to (5.18). Furthermore, by employing Equation (5.13), we can guarantee that we’ve set a nuclear core under the chosen valence space. Since the mathematics at the 3N level is highly complex, we’ll use the two-body truncation with the above equations in what’s known as the IM-SRG(2) formulation \([10, 150]\). However, we can still rest assured that 3N interactions have been included in our calculations.

5.3.1 Hartree-Fock Step

There is an important criterion about the nuclear core that we neglected to mention in the above discussion of normal ordering: Assumption 3. In particular, we want to make sure that the core is inert. That is, when taking all the single-particle oscillator basis states and using a Slater determinant to build a nuclear wave-function for the core, we want to make sure it is as close the ground state as possible. In IM-SRG \([135, 137]\), this is typically accomplish by using a Hartree-Fock wave-function for the In-Medium reference state:

\[
|\Psi_0\rangle \rightarrow |\Psi_{HF}\rangle
\]

Hence, we’ll use a Hartree-Fock variational step (see Section 2.1.4) before normal ordering can be calculated in IM-SRG. This will also ensure that our oscillator basis states transform into single-particle wave-functions which realistically match our choice of interaction.

5.4 The Magnus Formulation

In practice, implementing Equations (5.2), (5.7), and (5.12) is not always feasible because: the ODEs may become stiff, the advanced numerical integrations needed impose large memory costs,\(^*\) and solving for any additional operators requires another set of non-linear coupled ODEs to be solved. Furthermore, it is unclear how to systematically truncate the solution for the unitary matrix in Equation (5.8) under the \( s \)-ordering, and any such truncations will inevitably induce non-unitarity. These non-unitary resolution errors ultimately defeat the purpose of preserving observables under the SRG. To rectify these issues, we’ll use what is known as the “Magnus formulation”\(^†\) of IM-SRG \([149]\).

The first step to this formulation is to ask: how can we construct the unitary matrix necessary to similarity transform the Hamiltonian (and alike), in a computationally tactical way? The idea is to take the form of the unitary matrix as follows

\[
U_s = e^{i\Omega(s)} \text{ such that, } \Omega^\dagger(s) = -\Omega(s) \text{ and, } \Omega(0) = 0 \quad (5.20)
\]

\(^*\)which is especially a problem for larger model spaces

\(^†\)One would expect that, upon the continuing success of this “Magnus” implementation, it will soon be referred to as the “Morris” or “MPB formulation.”
5.4. The Magnus Formulation

It can be proven that this form exists as a solution to the linear system* of ODEs in Equation (5.8) [151]. The latter condition guarantees that $U_{s=0} = 1$ and hence $\hat{H}_{s=0} = \hat{H}$. But now that we’ve introduced more information in terms of $\Omega(s)$, we must find a suitable way of finding it. By generalizing Equation (5.8), one can construct the following ODE

$$\frac{d\Omega(s)}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} \text{ad}^k_{\Omega(s)}[\eta_s] = \eta_s + \frac{1}{2}[\Omega, \eta_s] + \frac{1}{12}[\Omega, [\Omega, \eta_s]] + \ldots$$

(5.21)

where $B_k$ are the Bernoulli numbers,† and we’ve introduced the shorthand notation for the recursively defined nested commutators for the square matrices $L$ (left) and $R$ (right)

$$\text{ad}^k_L[R] = [L, \text{ad}^{k-1}_L[R]] \quad \text{where} \quad \text{ad}^0_L[R] = R$$

(5.22)

As discussed previously in Section 5.2.2, we’ll take $\eta_s$ as the White generator.

So how does the introduction of Equation (5.20) possibly help us with our original task of using the SRG on the Hamiltonian? We see that the condition $\Omega^\dagger(s) = -\Omega(s)$ in combination with (5.2) gives us the innocuous modification

$$\hat{H}_s = e^{\Omega(s)} \hat{H} e^{-\Omega(s)}$$

(5.23)

From this point, one may use the Baker-Cambell-Hausdorff (BCH) formula on Equation (5.23) to obtain

$$\hat{H}_s = \sum_{k=0}^{\infty} \frac{1}{k!} \text{ad}^k_{\Omega(s)}[\hat{H}] = \hat{H} + [\Omega, \hat{H}] + \frac{1}{2}[\Omega, [\Omega, \hat{H}]] + \ldots$$

(5.24)

where we’ve used the same notation as defined in Equation (5.22). Now we can see the advantage of the Magnus formulation! We’ve effectively traded the cumbersome ODE in Equation (5.7) with a set of nested commutators for the Hamiltonian, in what is known as the “Magnus flow equation” (5.24), and the new ODE from (5.21).

It turns out that all we will need to solve the ODE in Equation (5.21) is a first-order forward Euler solver [149]. This will greatly cut memory costs when using IM-SRG, particularly for medium mass nuclei with large model spaces. Then, many computationally efficient diagrammatic methods for solving nested commutators can be exploited to SRG evolve the Hamiltonian via the Magnus flow equation. Furthermore, we can systematically truncate Equation (5.21) and (5.24), thus minimizing any non-unitarity induced in $U_s$. Thusly, the Magnus formulation introduces significant memory savings, avoids problems with stiff ODEs, and gives a way to systematically truncate the series sums whilst optimizing for unitarity loss.

The next pressing question is, then, how can we accomplish appropriate truncations? The current technique is the so-called “Magnus(2) truncation,” in conjunction with IM-SRG(2)

---

*it’s considered a system in terms of the matrices (mathematical operators) involved
†defined such that $B_1 = +1/2$
5.4. The Magnus Formulation

(described in Section 5.3 above). That is, it has been found empirically “that the magnitude of terms [in Equation (5.21) and (5.24)] decreases monotonically in \( k \) for all systems studied thus far.” [149] So, for some tolerances, \( \epsilon_{\text{deriv}} > 0 \) and \( \epsilon_{\text{BCH}} > 0 \), we can truncate the sum of nested commutators at the \( k \)-th term where

\[
\left| \frac{B_k \| \text{ad}_{\Omega(s)}^k [\eta] \|}{k! \|\Omega\|} \right| < \epsilon_{\text{deriv}}
\]

for Equation (5.21), and

\[
\left| \frac{\| \text{ad}_{\Omega(s)}^k [\tilde{H}] \|}{k! \|\Omega\|} \right| < \epsilon_{\text{BCH}}
\]

for Equation (5.24). The norms on the respective matrices are taken as the Frobenius norm

\[
\|\Omega\| = \sqrt{\sum_{ij} |\Omega_{ij}|^2} = \sqrt{\text{Tr}(\Omega \cdot \Omega^\dagger)}
\]

and it is commonly found that a wide range in \( \epsilon \)-tolerance values yields similar final results.

Now, as in Section 5.2.3, we may SRG any other operator of interest by using the same unitary matrix, \( U_s = e^{\Omega(s)} \), as we did for the Hamiltonian. Thus, upon the application of the BCH formula, we obtain the analog to Equation (5.24) for an arbitrary operator

\[
\tilde{O}_s = \sum_{k=0}^{\infty} \frac{1}{k!} \text{ad}_{\Omega(s)}^k [\tilde{O}] = \tilde{O} + [\Omega, \tilde{O}] + \frac{1}{2} [\Omega, [\Omega, \tilde{O}]] + \ldots
\]

with a similar truncation as in Equation (5.26). In this sense, we can now handle the calculation of any nuclear observable without having to solve an additional set of ODEs, as was required with Equation (5.12). Hence, we’ve translated the problem of solving multiple systems of (potentially stiff) ODEs for \( \tilde{H}_s \) and any \( \tilde{O}_s \) into solving one (Euler solvable) ODE for \( \Omega(s) \) and a BCH summation for Equation (5.24) and (5.27), whilst minimally violating unitarity. Overall, these non-perturbative equations for the nuclear many-body problem will require a numerical treatment, which we present in the next chapter.
Chapter 6

Numerical Methods

This chapter will cover the numerical methods that we will use in order to obtain the results of this research (see Chapter 7). In particular: \texttt{imsrg++} is used to evolve nuclear operators, via the theory of VS-IM-SRG; \texttt{NuShellX@MSU} is used to create realistic wave-functions of nuclear states, within the framework of the ShM; and \texttt{nutbar} bridges the latter two codes to make one-body transition densities (OBTDs) and two-body transition densities (TBTDs), to finally arrive at nuclear matrix element predictions. We’ll also detail how the $M^{
u
u}$ TBMEs were calculated computationally, within \texttt{imsrg++}.

6.1 \texttt{imsrg++}

To perform the valence space IM-SRG evolution of the Hamiltonian, and any additional desired observables, as described in Chapter 5, we’ll use a software developed by Dr. Ragnar Stroberg\textsuperscript{*} entitled \texttt{imsrg++}. It is written primarily in \texttt{C++}, using features from \texttt{C++11} with \texttt{python} bindings, and the libraries: \texttt{GSL},\textsuperscript{†} \texttt{BOOST},\textsuperscript{‡} \texttt{Armadillo},\textsuperscript{§} \texttt{OpenBLAS},\textsuperscript{¶} and \texttt{OpenMP},\textsuperscript{¶} among others. It is maintained by Dr. Stroberg under a GNU Public License,\textsuperscript{†} and stored in the \texttt{git} repository located at:∥ \texttt{https://github.com/ragnarstroberg/imsrg}.

This software has been highly successful for valence space IM-SRG calculations [135, 137]. Its source files are well organized and easy to compile in a Linux environment. Together, they perform all the relevant mathematics described in this dissertation, such as: angular momentum coupling (see Appendix A), the Hartree-Fock step (see Section 2.1.4), normal ordering (see Section 5.3), TBME construction (as in Chapter 4), and of course IM-SRG evolution (see Chapter 5). Furthermore, it comes equipped with many operators (located in the \texttt{imsrg_util} namespace), from electromagnetic observables to nuclear radii to beta decay. However, NMEs cannot be produced directly from it, since it needs to interface (see Section 6.1 further below) with a ShM code (see Section 6.2 directly below).

\textsuperscript{*}Dr. Stroberg was Dr. Jason D. Holt’s post-doctoral collaborator at TRIUMF for the majority of this dissertation research on double-beta decay. He is missed.

\textsuperscript{†}GNU Public License: \url{http://www.gnu.org/licenses/gpl.html}

\textsuperscript{‡}BOOST Software License: \url{http://www.boost.org/users/license.html}

\textsuperscript{§}Mozilla Public License: \url{https://www.mozilla.org/en-US/MPL/2.0/}

\textsuperscript{¶}BSD License: \url{https://opensource.org/licenses/BSD-3-Clause}

∥this is not necessarily a permanent link, contact Dr. Stroberg for maintenance issues
6.2 NuShellX@MSU

To construct a NME, we’ll need the appropriate wave-function information to build the OBTDs and TBTDs of Equation (C26) and (C33). That is, we’ll require the final nuclear state, |f⟩, and the initial nuclear state, |i⟩, to make

\[ \langle \eta_f J_f | [\hat{c}_a \otimes \hat{c}_b]_L | \eta_i J_i \rangle \quad \text{and} \quad \langle \eta_f J_f | [\hat{c}_a \otimes \hat{c}_b]_{ab} \otimes [\hat{c}_c \otimes \hat{c}_d]_{cd} \otimes \hat{L} | \eta_i J_i \rangle \]

for one-body operators (see Section C.2) and two body operators (see Section C.3), respectively.*

We’ll build these eigenvectors using the shell model code known as NuShellX@MSU [152]. To perform the diagonalization of the Hamiltonian for low-lying states in the nuclear ShM, NuShellX uses the Lanczos algorithm [153]. It’s constructed in PN formalism and J-scheme, which corresponds with how we’ve treated our OBMEs and TBMEs throughout this text. NuShellX also comes with a library of interaction files suitable for many valence spaces, but one can interface their own interactions, which we do from imsg++ using SRG evolved χEFT input files.

6.3 nutbar

In order to calculate the OBTDs and TBTDs via the wave-functions from NuShellX, and then combine them with the IM-SRG evolved OBMEs and TBMEs to produce NMEs,† we’ll employ a code called nutbar. It is maintained by Dr. Stroberg at the git repository location:‡

https://github.com/ragnarstroberg/nutbar. nutbar is an acronym which stands for: NuShellX Transitions from Binary Arrays.§ It’s a necessary interface between NuShellX and imsg++, since the former does not provide the ability to calculate TBTDs for spherical tensors. Furthermore, IM-SRG will push information between one-body and two-body matrix elements (see Section 5.3). Due to this fact, nutbar is also used to keep the OBTDs consistent.

6.4 Two-Tiered Adaptive \( M^{0\nu} \) TBMEs

For the \( M^{0\nu} \) TBMEs (see Chapter 4), we first integrate with respect to \( r \) (see Equation (4.64) for instance) and then, after performing the summations for the relevant augmented operators in Equations (4.46), (4.50), and (4.31), we’ll integrate with respect to \( q \) for Equation (4.71). In practice, this turned out to be more awkward than desired. First, it is clear that Equation (4.71) will require an adaptive integration technique over the interval \([0, \infty)\), so we turned to the GNU Scientific Library for integration functions [154]. Since the accuracy of the integral with respect to \( r \), which is parameterized by the relative quantum numbers \( n_r, I_r, n'_r, I'_r, \)

---

*both have been written for a rank L spherical tensor operator, to get the amplitude \( \langle f | \hat{T}_L | i \rangle \)
†via Equation (C26) and (C33)
‡this is not necessarily a permanent link, contact Dr. Stroberg for maintenance issues
§NuShellX stores its wave-function data in binary
affects the convergence of the $q$ integration - for higher lying orbits we would often receive the `GSL_EDIVERGE` error:

\[\text{the integral is divergent, or too slowly convergent to be integrated numerically.}\]

To make matters more complicated, for higher sets of the relative quantum numbers, Equation (4.64) and alike\(^\ast\) would start to fail. This was because the Gamma functions in both the normalization constant and the generalized binomial coefficients of Equation (4.64) would blow up, even when implementing clever and efficient uses of the `tgamma_ratio` function from `BOOST`.

To rectify these issues, we developed a two-tiered adaptive integration scheme, as illustrated in Table 6.1. We called this “two-tiered” since we `adaptively` choose which `adaptive` integration methods to use based on the values of $n_r, l_r, n'_r, l'_r$. Ultimately, this scheme solved all the issues presented above. However, to be properly implemented, we needed to expand the `imsrg++` framework with a package we named `NDBD.hh` and `NDBD.cc,\(^\dagger\)` which represents a modest 1,300 lines of highly optimized object-oriented code written in `C++`. The `NDBD` class (which stands for `Neutrinoless Double-Beta Decay`) is exclusively used in `imsrg_until.cc` to build the TBMEs, and required slight modifications to `imsrg++.cc` and alike. It also takes advantage of symmetries like $I(n_r, l_r, n'_r, l'_r) = I(n'_r, l'_r, n_r, l_r)$ and more, and employs parallelization\(^\‡\) and caching techniques for memory cost reduction and significant speed increases.

<table>
<thead>
<tr>
<th>$n_r, l_r, n'_r, l'_r$</th>
<th>$dr$</th>
<th>$dq$</th>
</tr>
</thead>
<tbody>
<tr>
<td>[4, 8, 4, 8]</td>
<td>analytic</td>
<td>QAGIU</td>
</tr>
<tr>
<td>[10, 10, 10, 10]</td>
<td>analytic</td>
<td>QAG</td>
</tr>
<tr>
<td>($\infty$, $\infty$, $\infty$, $\infty$)</td>
<td>QAGIU</td>
<td>QAG</td>
</tr>
</tbody>
</table>

Table 6.1: Two-tiered integration scheme for $M^{0\nu}$ TBMEs. The integration type is first used with respect to $r$ (relative distance coordinate), and then $q$ (neutrino momentum). This set of integrations for $(dr, dq)$ are used for the relative quantum numbers $n_r, l_r, n'_r, l'_r$ for values less than or equal to those found in the first column of the table. The analytic integration uses either Equation (4.64) or (4.70) with (4.62), depending on whether or not SRCs are included. QAG [155] and QAGIU [156] adaptive integration techniques are from `GSL`. This scheme was found to be acceptable for $e_{\text{max}} \leq 10$, and we expect it to work beyond this.

Note that the values for the relative quantum numbers\(^\S\) in the first column of Table 6.1 were found by trial and error, and they (if not the whole structure of the table) may need to be changed with evolving versions of the code. We found that the first integration to fail was for $dq$, using the highly adaptive QAGIU algorithm (see QAGIU in Section 6.4.1 below).

\(^\ast\)Equation (4.70) and (4.62) for the inclusion of SRCs
\(^\dagger\)For details on this version of `imsrg++`, please contact me at: cgpayne@triumf.ca. At the time of writing, it has not been pushed to the remote `GitHub` repository at [1].
\(^\‡\)via OpenMP
\(^\S\) $n_r$ and $n'_r$ will run from 0 to $e_{\text{max}}$, and $l_r$ and $l'_r$ will run from 0 to $2 \cdot e_{\text{max}}$. To see this simply maximize the limits from Equation (D21).
6.4. Two-Tiered Adaptive $M^{0
u}$ TBMEs

Hence, for relative orbits greater than $(n_r, l_r, n'_r, l'_r) = (4, 8, 4, 8)$ we switched from QAGIU to the QAG algorithm (see QAG in Section 6.4.1 below). Since QAG requires a finite interval of integration, we found that taking $a = 0$ MeV to $b = 2,500$ MeV was sufficient to approximate a semi-infinite interval, since all integrands would have decayed in this range. However, at roughly $(n_r, l_r, n'_r, l'_r) = (10, 10, 10, 10)$ the analytic formula for the $r$ integration would fail due to reasons previously mentioned. This is disappointing, since an analytic formula for an integral is more computationally efficient than an adaptive method. Nonetheless, QAGIU is optimized, so we switch to this to handle the RBMEs of Equation (4.51) alternatively adaptively at this point.

6.4.1 Integration Techniques from GSL

Before presenting the final results from these numerical methods for the neutrinoless double-beta decay of Calcium-48, we’ll briefly describe the adaptive integration methods that we used from the GNU Scientific Library [154]. Note that, for both the gsl_integration_qagiu and gsl_integration_qag functions from GSL, we found $(\text{limit}, \text{epsabs}, \text{epsrel}) = (1e^{-4}, 1e^{-7}, 1e^{-5})$ to be appropriate for the integration with respect to $r$, and $(\text{limit}, \text{epsabs}, \text{epsrel}) = (N_{\text{threads}} 	imes 1e^{-4}, 1e^{-7}, 1e^{-4})$ to be appropriate for the integration with respect to $q$. The epsabs and epsrel terminate the integration (and subsequently define “convergence”) when

$$\left| F(x_i) - F(x_{i-1}) \right| \leq \epsilon_{\text{abs}} \text{ or, } \left| 1 - F(x_i)/F(x_{i-1}) \right| \leq \epsilon_{\text{rel}}$$

respectively. $F(x_i)$ represents the sequence of summed integrals of some integrand, $f(x)$, on the set of adaptively chosen $\{x_i \text{ s.t. } i \in \mathbb{N}_0\}$.

QAGIU

To integrate a function, $f(x)$, over the interval $[a, \infty)$, the QAGIU algorithm [156] maps the domain to $(0, 1]$ using the coordinate transformation $x = a + (1 - t)/t$, giving

$$\int_{a}^{\infty} dx f(x) = \int_{0}^{1} dt \frac{f(a + (1 - t)/t)}{t^2}$$

It is clear that the integrand on the RHS may have singularities. Hence, from this point, the QAGS algorithm [157] is implemented, which is an adaptive method that can handle integrable singularities. QAGS uses adaptive bisection along with the Gauss-Kronrod 21-point quadrature [158], and the Wynn’s $\epsilon$-method [159] to speed up the convergence.

QAG

To integrate a function, $f(x)$, over the interval $[a, b]$, the QAG algorithm [155] splits the domain into subintervals and applies a Gauss-Kronrod quadrature [158]. We opted to use a 61-point rule ($\text{key} = 6$). The algorithm focuses on subintervals where the integration is less well behaved, and then applies adaptive bisections.

*alternatively, Equation (4.67) when SRCs are desired
Chapter 7

Results

In Chapter 2, we gave a comprehensive review on all the basic elements needed to construct nuclear theory and the valence space IM-SRG framework from Chapter 5. Additionally, we reviewed the physics and current developments of double-beta decay in Chapter 3, which lead to a thorough derivation of the $M^{0\nu}$ TBMEs in Chapter 4. With this footwork in place, we are now finally ready to present the results of this research project, which were computed using the numerical methods of Chapter 6.

First we will put forth results for $2\nu\beta\beta$ and then for $0\nu\beta\beta$, both for the nucleus Calcium-48, since its doubly magic shell closure makes it an ideal medium-mass nuclei to calibrate our many-body method with, and it is the lightest double-beta decay candidate. Accordingly, we’ll take the valence space to be the $pf$-shell ($1p_{3/2}, 1p_{1/2}, 0f_{7/2}$, and $0f_{5/2}$ orbits). To demonstrate that imsr++ is working as expected and that we have NMEs which are comparable with the double-beta decay community, we will benchmark based on the following principle:

Remark 7.1
Running VS-IM-SRG without any Magnus evolution, In-Medium normal ordering, or Hartree-Fock step (hence, using a pure harmonic oscillator basis) $\implies$ we should be able to match with NMEs from standard ShM results using phenomenological interactions.

With this remark in hand, we can check that we’ve properly solved for the $M^{2\nu}$ OBMEs (see Section 3.1.3) and $M^{0\nu}$ TBMEs (see Section 4.6), which represents a extensive mathematical undertaking. From there, we’ll evolve the NMEs using VS-IM-SRG with the Magnus(2) formulation (see Section 5.4) and $\chi$EFT interactions, and compare the results with our benchmarks. As discussed in Section 5.2.1 and 5.3, the main difference between the benchmarked NMEs and our evolved results will be the inclusion of ab initio interactions and 3N physics.

7.1 $2\nu\beta\beta$ NME for $^{48}\text{Ca}$

Before we can test whether VS-IM-SRG is capable of producing neutrinoless double-beta decay NMEs which are more or less reliable than current values from other methods, we must demonstrate that $2\nu\beta\beta$ is under control within the theoretical framework. This is a convenient course of action using Calcium-48, since we know that it undergoes standard double-beta decay (see Section 3.1.1 and Example 3.1). Also, since no neutrinoless mode has ever been measured,
7.1. 2νββ NME for 48Ca

calibrating with respect to 2νββ is the first reasonable step. Furthermore, neither 2νββ nor 0νββ have been modelled using a fully ab initio approach, so it is imperative that we benchmark both these decays against the current phenomenology.

To calculate the 2νββ NMEs, we’ll use Equation (3.14), printed again below for convenience, with a summation over \( k = 1 \) to 250 intermediate excited states. To obtain the individual Gamow-Teller NMEs in the numerator of Equation (7.1), we’ll use nutbar (see Section 6.3) to construct Equation (C26) using the OBMEs from (2.44). Note that the excitation energies of 48Sc, and its 6\(^+\) ground state, will depend on the many-body method used, likewise with the NMEs. This makes the choice of interaction somewhat tricky for the case of two-neutrino double-beta decay, since such an interaction must be tailored to produce both: good energy levels and good GT transitions. For now, we’ll leave this point for future considerations.

\[
M^{2\nu}(48\text{Ca}^{0+} \rightarrow 48\text{Ti}^{0+}) = \sum_{k=1}^{250} \frac{\langle 48\text{Ti}^{0+} | \hat{\sigma}_\tau | 48\text{Sc}^{1+}_k \rangle \langle 48\text{Sc}^{1+}_k | \hat{\sigma}_\tau | 48\text{Ca}^{0+} \rangle}{E'_k - E(48\text{Sc}^{6+}_{g.s}) + \delta E_1 + X [\text{MeV}]} \quad (7.1)
\]

\[
\delta E_1 = \begin{cases} 
2.5173 \text{MeV} - [E'_1 - E(48\text{Sc}^{6+}_{g.s})], & \text{for phenomenology} \\
0, & \text{for ab intio}
\end{cases}
\]

\[
X = \begin{cases} 
1.859700017, & \text{for phenomenology} \\
1.348701071, & \text{for ab intio}
\end{cases}
\]

One last detail to mention before we proceed is that, for the phenomenological case of modelling 2νββ, it is common to shift \( E_k \), for \( \forall k \), such that the lowest lying \((k = 1)\) excited 1\(^+\) state matches the experimental value. In Equation (7.1), we’ll include this correction by adding “\( \delta E_1 \)” into the denominator. The lowest lying excited 1\(^+\) state of 48Sc is at 2.5173 MeV,\(^\ast\) which we obtained from [74]. The \( X \) term in the denominator is simply the mass contribution, as calculated for Equation (3.14). The difference between the phenomenology and our ab initio calculations will be by one \( m_e \), which we believe to be an non-negligible error.

7.1.1 Phenomenological Benchmarking (2νββ)

To benchmark \( M^{2\nu} \), we’ll apply Remark 7.1 and compare against [71, 73]. The results are plotted in Figure 7.1. As we can see, when we set the quenching factor (see Section 3.1.4), \( q_f \), to 0.77,\(^\dagger\) the imsr++ and nutbar codes precisely reproduce the running sum of the \( M^{2\nu} \) NME from [73]. The match happens because no Magnus evolution was used and all other parameters are matched: 10.49 MeV basis frequency, \( pf\) -shell valence space, GXPF1A phenomenological interaction [31, 32], etc. This should be no surprise, since the cited literature values were also calculated using NuShellX (see Section 6.2) and a valence space approach.

Additionally, both panels show that convergence happens as long as the sum is taken to run over the Gamow-Teller resonances at \( \approx 6 \text{ MeV} \). We report our phenomenological result as

\(^\ast\)relative to its 6\(^+\) ground state
\(^\dagger\)coloured as orange in the Figure 7.1
7.1. $2\nu\beta\beta$ NME for $^{48}\text{Ca}$

Figure 7.1: Benchmarking for the two-neutrino double-beta decay NME of $^{48}\text{Ca}$ using a $pf$-shell valence space and the GXPF1A interaction. The oscillator basis frequency was taken as $\hbar\omega = 10.49\text{MeV}$ from Equation (2.6) to match with [126]. We’ve plotted the NME as the running sum via Equation (7.1) as a function of the intermediate nuclei’s excitation energies (relative to the $6^+$ ground state). The left panel shows our results by running imsr++ without any IM-SRG evolution by setting the maximum flow parameter to $s_{\text{max}} = 0$, in accordance with Remark 7.1. The right panel has been taken from [73] and adapted by highlighting the GXPF1A result in orange ($q_f = 0.77$), for clarity. The red solid line represents the expected NME from experiment, see Equation (3.5). To reproduce the phenomenology in the right panel, we adjusted $1.348701071\text{MeV} \rightarrow 1.859700017\text{MeV} \approx 1.9\text{MeV}$ in Equation (7.1), which is a convention used in the literature which we believe to be erroneous (hence this adjustment will not be used for the ab initio results below).

\[
M^{2\nu}=\begin{cases} 0.09080\text{MeV}^{-1}, & q_f=1 \\ 0.05384\text{MeV}^{-1}, & q_f=0.77 \end{cases}
\tag{7.2}
\]

which matches the values from [71, 73]. However, without quenching ($q_f = 1$), this result is clearly much larger than the experimentally expected value of $0.03846\text{MeV}^{-1}$, and motivates the desire to quench the $2\nu\beta\beta$ in correspondence with single-beta decay (see Section 2.3.4). In conclusion, we’ve shown that imsr++ can properly reproduce the current phenomenology,* and so our code has been appropriately benchmarked for $2\nu\beta\beta$.

---

*Note that the first excited states were corrected using $\delta E_1$ in Equation (7.1), and without this correction we were not able to precisely reproduce the phenomenology.
7.1.2 VS-IM-SRG Using the EM 1.8/2.0 Interaction ($2\nu\beta\beta$)

We now use the Magnus(2) evolution with the so-called “EM 1.8/2.0” interaction \cite{38}, and plot the results in Figure 7.2. As with the phenomenological benchmarking, we see that convergence has taken place, since we’ve summed over enough intermediate nuclear states to overcome the GT resonance at $\approx 6\text{ MeV}$. However, in comparison with phenomenology (reprinted in the left panel), the evolved $M^{2\nu}$ is much lower! It even dips somewhat below the experimentally expected result (red solid line). This suggests that an ab initio calculation of nuclear double-beta decay includes significant contributions, such as higher-order many-body forces.

Many interactions do not properly reproduce the energy spectra of nuclei from first principles, but such an interaction is needed for Equation (7.1) because of the energy terms in the denominator. Hence, it should be stressed that the choice of the EM 1.8/2.0 interaction was crucial for this calculation. In fact, this interaction was so successful in energy calculations that we found no measurable difference between using a correction to the first excited states (as discussed beneath Equation (7.1) above) and running them fully ab initio. This gives credence to fact that the EM 1.8/2.0 interaction can be trusted for $0\nu\beta\beta$ calculations.

\*This interaction gets its name since it’s an SRG evolution of the $\chi$EFT from Entem and Machleidt (EM) \cite{160} with the LECs labelled as 1.8/2.0. It has been so successful in ab initio calculations for medium mass nuclei that it is sometimes referred to as the “magic” interaction.
We report our ab initio result as

\[
M^{2\nu} = \begin{cases} 
0.02977 \text{ MeV}^{-1}, & q_f = 1, \text{ without MECs} \\
0.01180 \text{ MeV}^{-1}, & q_f = 1, \text{ with MECs}
\end{cases}
\]  

(7.3)

Notice that when we include meson exchange currents (MECs), the NME is suppressed even lower than desired. This is a conflicting result, since \(\chi\)EFT calculations including MECs may account for quenching \([52]\). Hence, we had hoped to see that the MECs would correct for the slight difference between the non-MEC result in Equation (7.3) and the experimentally expected value of 0.03846 MeV\(^{-1}\). It should be no surprise that this did not occur, however, since it is possible that important \(1^+\) intermediate states were not captured using this valence space approach. That is, we expect that there exist \(1^+\) states of \(^{48}\)Sc that would correct for the small difference between our quoted result and the experimental value, but such states lie outside the \(pf\)-shell valence space.

To test this idea in the future, we may: run a non-VS version of IM-SRG, or compare with a different many-body method which employs a large single-particle space. A collaborating group, under Dr. Gaute Hagen, uses the Coupled-Cluster (CC) theory, which can perform these types of calculations. Hence, in upcoming studies, this discrepancy will be resolved. In any case, an argument can be made that both results (with and without MECs) are still significantly closer to the experimentally expected value than previous calculations using phenomenological interactions and no quenching. Thus, we conclude that \(2\nu\beta\beta\) has been modelled well within the framework of VS-IM-SRG, and our following neutrinoless results are trustworthy. In fact, since \(0\nu\beta\beta\) employs the closure approximation, we need not worry about capturing all the intermediate states in this case - and any problems with the above results are not expected to translate to the following sections.

### 7.2 \(0\nu\beta\beta\) NME for \(^{48}\)Ca

To calculate the \(0\nu\beta\beta\) NMEs, we’ll use the formulae from Section 4.6, and nutbar (see Section 6.3) to construct Equation (C33). In particular, to obtain the GT, F, and T TBMEs, we’ll use Equation (4.71) with Equations (4.46), (4.50), and (4.31). Note that these TBMEs are reliant on many parameters, which the double-beta decay community have been somewhat inconsistent with. For example, the \(\mu_p - \mu_n\) is often set to 3.7,\(^*\) in order to compare with previous results in the literature, such as \([126]\). We will take the parameters from Table 7.1 below, and explicitly state whether the “outdated” or “updated” sets of parameters were used.

To produce the total \(M^{0\nu}\) NME, we need to calculate the three decay transitions under the

---

\(^*\)If the proton and neutron were elementary particles, then \(\mu_p = 1\) and \(\mu_n = 0\) and therefore \(\mu_p - \mu_n = 1\). However, the measured value is \(\approx 4.7\), since nucleons are composed of quarks. Sometimes this experimental parameter is thought of in terms of its deviation from the classical theoretical expectation, hence the confusion between 4.7 and 3.7. Surely, 3.7 is erroneous in the context of \(0\nu\beta\beta\).
7.2. $0\nu\beta\beta$ NME for $^{48}\text{Ca}$

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_0^{\text{cl}}(^{48}\text{Ca})$</td>
<td>[MeV]</td>
<td>7.72</td>
</tr>
<tr>
<td>$m_p$</td>
<td>[MeV]</td>
<td>938.2720814</td>
</tr>
<tr>
<td>$m_\pi$</td>
<td>[MeV]</td>
<td>139.57018</td>
</tr>
<tr>
<td>$\mu_p - \mu_n$</td>
<td>[$\mu_N$]</td>
<td>3.7</td>
</tr>
<tr>
<td>$g_{V,0}$</td>
<td>[unitless]</td>
<td>1</td>
</tr>
<tr>
<td>$g_{A,0}$</td>
<td>[unitless]</td>
<td>1.25</td>
</tr>
<tr>
<td>$\Lambda_V$</td>
<td>[MeV]</td>
<td>850</td>
</tr>
<tr>
<td>$\Lambda_A$</td>
<td>[MeV]</td>
<td>1086</td>
</tr>
<tr>
<td>$r_0$</td>
<td>[fm]</td>
<td>1.2</td>
</tr>
<tr>
<td>$\hbar \cdot c$</td>
<td>[MeV·fm]</td>
<td>197.3269718</td>
</tr>
<tr>
<td>$m_N$</td>
<td>[MeV]</td>
<td>938.9187474</td>
</tr>
</tbody>
</table>

Table 7.1: Values of $M^{0\nu}$ parameters. Two sets of different parameters will be used: one for benchmarking (third column), and one for the VS-IM-SRG evolution (fourth column). The choice of closure energy is nuclei-dependent, and we’ve taken it as 7.72 MeV for $^{48}\text{Ca}$, which has become a standard - although there is some debate as to what makes the optimal closure energy [118], which should be researched more in the future. The only differences between the outdated and updated parameters have been highlighted in red, and we’ll see that they indeed make an effect, which makes benchmarking difficult.

\[ M^{0\nu} = M^{0\nu}_{\text{GT}} = \left( \frac{g_V}{g_A} \right)^2 M^{0\nu}_F + M^{0\nu}_T \]  

Notice that the factor in front of the Fermi term in the sum is there to make it independent of the value of the axial-vector coupling constant - which changes as experiments become more precise. First we will conduct the phenomenological benchmarking, as was done in Section 7.1.1 above, and then we will present results using two different $\chi$EFT interactions, both with and without the inclusion of short-range correlations (SRCs).

### 7.2.1 Phenomenological Benchmarking ($0\nu\beta\beta$)

To benchmark $M^{0\nu}$, we’ll apply Remark 7.1 and compare against [71, 118, 126, 133]. To make a proper parallel between said references, we’ll use the parameters listed in the “outdated” column of Table 7.1; and then, to see what difference the corrected parameters induce, we’ll also run results for the “updated” column. We’ll see that the use of these different parameters make a small difference, hence contrasting any results from Section 7.2.2 or 7.2.3 with these benchmarks is valid. The results are tabulated in Table 7.2 below.
7.2. $0\nu\beta\beta$ NME for $^{48}\text{Ca}$

<table>
<thead>
<tr>
<th>SRCs:</th>
<th>none</th>
<th>AV18</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameters:</td>
<td>Outdated</td>
<td>Updated</td>
</tr>
<tr>
<td>$M_{GT}^{0\nu}$</td>
<td>0.6767</td>
<td>0.7090</td>
</tr>
<tr>
<td>$M_{F}^{0\nu}$</td>
<td>−0.2074</td>
<td>−0.2074</td>
</tr>
<tr>
<td>$M_{T}^{0\nu}$</td>
<td>−0.06954</td>
<td>−0.07479</td>
</tr>
<tr>
<td>$M^{0\nu}$</td>
<td>0.7400</td>
<td>0.7628</td>
</tr>
</tbody>
</table>

Table 7.2: Benchmarking for the neutrinoless double-beta decay NME of $^{48}\text{Ca}$ using a pf-shell valence space and the GXPF1A interaction. The oscillator basis frequency was taken as $\hbar\omega = 10.49\text{MeV}$ from Equation (2.6) to match with [126]. We ran imsr++ without any IM-SRG evolution by setting the maximum flow parameter to $s_{\text{max}} = 0$, in accordance with Remark 7.1. Both sets of parameters from Table 7.1 were used, along with SRCs set to none or the AV18 parameterization. Note that the concept of a model space size ($e_{\text{max}}$) is irrelevant here, since no decoupling will occur without running the IM-SRG (see Section 5.1.1). However, since an $e_{\text{max}}$ must be set to run the imsr++ code, by construction, multiple $e_{\text{max}}$’s were checked and they all gave identical results, modulo random pivots used for the Lanczos algorithm in NuShellX (which changed the results negligibly to the 6th significant digit).

Without SRCs (Benchmarking)

First, we’ll discuss the results in Table 7.2 without any SRCs (see Section 4.5.1). $M^{0\nu}$ is reported in the literature as: 0.711, from Table 3 of [126]; and 0.833, from Table 1 of [133].* [126] used the outdated parameters from Table 7.1, hence why this value matches well with our reported value of 0.7400 from Table 7.2. We propose that the slight difference in these values (0.711 and 0.7400) originates from [126] using a different ShM code. This builds our confidence that we have properly coded $0\nu\beta\beta$ into the imsr++ framework.

We could not reproduce the value from [133], since the GXPF1B interaction is currently not available within NuShellX using the PN formalism. Nonetheless, their value is still close to our reported result of 0.7628 from Table 7.2. Note that we’ve assumed they have used the updated parameters listed in Table 7.1, since it is not made explicit in the text, but it is a recent publication. The authors have used a closure energy of 0.5 MeV, and they state that using 7.72 MeV would reduce their value by roughly 5%, giving 0.792. This is hopeful, since it is reasonable to presume that the difference between our NME and that from [133] originates from the difference between the GXPF1A versus GXPF1B interactions. More conclusive evidence that we have properly benchmarked $0\nu\beta\beta$ will be discussed in the following section.

The differences between using the outdated and updated parameters from Table 7.1 are approximately: 5% for the Gamow-Teller, 0% for the Fermi, and 8% for the Tensor. This yields a 3% difference in the total NME, for the phenomenology without SRCs - which is negligible compared to the closure approximation (see Assumption 2 and Section 3.3.4). Note that the 0% difference in the Fermi term is to be expected, since this transition has no axial-vector or magnetic moment dependence.

*note that the GXPF1B interaction was used in the latter publication
With SRCs (Benchmarking)

Now we’ll discuss the results from Table 7.2 including the SRCs; in particular, we choose the AV18 parameterization of the Jastrow-type function in Equation (4.66). That is, we’ll set $a, b, c$ to the values found in row 1 of Table 4.1, and apply Equation (4.70) with (4.62) for the $M^{0\nu}$ TBMEs. $M^{0\nu}$ is reported in the literature as: 0.779, from Table 3 of [126]; 0.82, from Table 2 of [71]; 0.729, from Table 1 of [118]; and 0.801, from Table 1 of [133].\footnote{It is encouraging to see that all these values are in the same ballpark, and the small variations can be accounted for by the different methods and inputs used.}

The best match with our result of 0.7230 from Table 7.2 are those from [118]. To be explicit with the comparison, see Table 7.3 below. The small difference between these values can be accounted for by the use of $g_A = 1.254$ in [118], whereas we used 1.27. Another source of error comes from the use of different integration techniques (see Section 6.4). Otherwise, this replication is precise, which is to be expected since we’ve duplicated the methods used in [118]; in contrast to [71, 126, 133]. From this, we conclude that the $0\nu\beta\beta$ TBMEs have been properly incorporated into our framework, and we can now confidently proceed to evolving the NMEs.

<table>
<thead>
<tr>
<th></th>
<th>Our Values</th>
<th>Values from [118]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M^{0\nu}_{GT}$</td>
<td>0.6735</td>
<td>0.676</td>
</tr>
<tr>
<td>$M^{0\nu}_{F}$</td>
<td>-0.2041</td>
<td>-0.204</td>
</tr>
<tr>
<td>$M^{0\nu}_{T}$</td>
<td>-0.07702</td>
<td>-0.077</td>
</tr>
<tr>
<td>$M^{0\nu}$</td>
<td>0.7230</td>
<td>0.729</td>
</tr>
</tbody>
</table>

Table 7.3: Comparison of the neutrinoless double-beta decay NMEs, for benchmarking. The first column of values has been taken from the fourth column of Table 7.2, and the second column of values are the “Closure” NMEs from Table 1 of [118]. This clearly shows that we have benchmarked $0\nu\beta\beta$ properly, and that [118]’s values are indeed independently reproducible.

It is also worth noting that the introduction of SRCs has made some effect. This total change of roughly 5% is arguably comparable to the use of the closure approximation, and so it can be said that SRCs may yield non-negligible contributions. However, this presents a new challenge, since many different sets of SRCs exist (see Table 4.1), and they each give different results, see [118, 123]. Hence, future work must be conducted with the purpose of definitively establishing which set of SRCs are optimal for $0\nu\beta\beta$.

7.2.2 VS-IM-SRG Using the EM 1.8/2.0 Interaction ($0\nu\beta\beta$)

Now that we know the $M^{0\nu}$ NMEs have been coded properly within the imsr++ framework, we can proceed with evolving them using the Magnus(2) formulation (see Section 5.4). This evolution will capture more of the induced many-body physics happening with in the pf-shell valence space (see Section 5.3), and hence it should give a more accurate NME than the standard phenomenological ShM calculations presented in Section 7.2.1. To ensure that we have a more
precise model of $0\nu\beta\beta$, we’ll exclusively use the updated set of parameters from the fourth column of Table 7.1. Coupled with an appropriate $\chi$EFT interaction, this is the first time that $0\nu\beta\beta$ has been calculated using a fully ab initio, non-perturbative method.

Since the EM 1.8/2.0 interaction [38] has been so successful, and it convincingly modelled $2\nu\beta\beta$ in $^{48}\text{Ca}$ within the $pf$-shell (see Section 7.1.2), we will start by using this as our interaction input. MECs, on the other hand, will not be included since their contributions to $0\nu\beta\beta$ have not been developed at this time, by any study. Since we use the closure approximation for $0\nu\beta\beta$, we need not worry about missing intermediate states as in $2\nu\beta\beta$, which we’ve proposed are the source of the difference between the experimental $M_{2\nu}$ and our evolved values.

**Without SRCs (EM 1.8/2.0)**

First, we’ll present results without any SRCs (see Section 4.5.1). They can be seen in Figure 7.3, along with an analysis of the convergence. These results clearly show that the inclusion of many-body physics, via a fully ab initio calculation, has decreased the total $0\nu\beta\beta$ NME by about 20%, in comparison with the phenomenological results from Table 7.2. Via Equation (3.18), we predict a half-life which is approximately 60% longer than the current phenomenology. From an experimental perspective, this is clearly not favourable, since more source material will be required. It is not clear if this extrapolates to heavier nuclei, and it should be stressed that no theoretical arguments exist which forbid the induced many-body physics from giving the opposite trend. Furthermore, MECs will make an appreciable effect. VS-IM-SRG calculations for heavier nuclei, and the inclusion of MECs, will be studied in future work.

**With SRCs (EM 1.8/2.0)**

Now we’ll present results including SRCs; in particular, we choose the AV18 parameterization of the Jastrow-type function in Equation (4.66). That is, we’ll set $a, b, c$ to the values found in row 1 of Table 4.1, and apply Equation (4.70) with (4.62) for the $M_{0\nu}^\text{TBMEs}$. They can be seen in Figure 7.4, along with an analysis of the convergence. A significant difference has been introduced by the inclusion of SRCs here. The evolved SRC NMEs are roughly 30% lower than the phenomenological SRC values from Table 7.2. Via Equation (3.18), this corresponds to a half-life which is 2 times longer than the phenomenology. As mentioned at the end of Section 7.2.1, however, more research is needed to develop a methodology for which SRC parameters are optimal, so any interpretation of these results is likely premature.

The evolved SRC values are approximately 20% lower those without any SRCs, in comparison to the 5% drop seen for the phenomenology. This is well beyond any error introduced by the closure approximation, and therefore it could be proposed that SRCs are indeed non-negligible for a VS-IM-SRG evolution. It is interesting to note that the convergence pattern seen in Figure 7.4 matches that seen in Figure 7.3, which provides evidence that any apparent convergence irregularities are actually consistent within the calculations - as opposed to being computational anomalies within the IM-SRG framework (see Equation (5.10), for instance).
7.2.3 VS-IM-SRG Using the 500/400 N$^3$LO+3N Interaction (0νββ)

Here, we’ll present results without any SRCs, and using a different interaction from Section 7.2.2 above. The purpose is twofold: we have access to more basis frequencies for this interaction to assess convergence, and it is important to check how using a different interaction will affect the NMEs overall. The interaction we choose here is referred to as “500/400 N$^3$LO+3N.”* The results can be seen in Figure 7.5, along with an analysis of the convergence.

Visually, it is much clearer that these calculations converge, as compared to those in Figure 7.3, since more basis frequencies were available using this interaction. Of course, if we would’ve had more basis frequencies for EM 1.8/2.0, the coloured lines would have approached each other in a similar manner, as $e_{\text{max}}$ increases. However, the speed of convergence is interaction dependant. Although it appears that these values converge faster than those from the EM 1.8/2.0 interaction, we choose to trust the latter NMEs more, since this interaction was better suited for the 2νββ calculations. Thus, the much lower NME of approximately 0.27 should not be interpreted physically - we only performed these calculations to check convergence.

7.2.4 Summary (0νββ)

Since we’ve developed the power to calculate 0νββ using imsrg++ in a general and efficient manner, we were able to present many results. Hence, for succinctness, in Table 7.4 we summarize our final results for neutrinoless double-beta decay. We may extrapolate our NME for 0νββ without SRCs as $M_{0\nu} \approx 0.6$. Remarkably, this value matches with that reported in Table 1 of [163], which used an interacting ShM approach with full calculations in the pf-shell that implemented: seniority truncations, nuclear currents, and took account for pairing affects.

<table>
<thead>
<tr>
<th>Interaction</th>
<th>SRC</th>
<th>$M_{0\nu}$ [MeV]</th>
<th>$\hbar\omega$ [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>EM 1.8/2.0</td>
<td>none</td>
<td>0.5663</td>
<td>0.6300</td>
</tr>
<tr>
<td>EM 1.8/2.0</td>
<td>AV18</td>
<td>0.4718</td>
<td>0.5219</td>
</tr>
<tr>
<td>500/400</td>
<td>none</td>
<td>0.2846</td>
<td>0.2649</td>
</tr>
</tbody>
</table>

Table 7.4: Summary of the VS-IM-SRG evolved neutrinoless double-beta decay NMEs of 48Ca using a pf-shell valence space. All of the entries are the total sum, $M_{0\nu}$, using the updated parameters from Table 7.1. Convergence is set at $e_{\text{max}} = 10$ (see Figures 7.3 to 7.5). Results using the EM 1.8/2.0 interaction are considered more trustworthy, as discussed in the text. The 500/400 N$^3$LO+3N interaction is only included to demonstrate the independence of NMEs as a function of $\hbar\omega$ at this $e_{\text{max}}$. The latter interaction’s results vary over $\approx 8\%$ with respect to $\hbar\omega$, and the former’s results vary over $\approx 11\%$; which is comparable to the closure approximation. The SRCs, induce a difference of $\approx 20\%$, and so they may be considered non-negligible.

We now print the figures referenced to throughout the text of this section.

*This interaction first appeared in [135]. In accordance with [162], a χEFT interaction was built from N$^3$LO for NN and N$^2$LO for 3N and then SRG evolved starting with $\Lambda_{\text{NN}} = 500$ MeV and $\Lambda_{3N} = 400$ MeV - hence the naming of the interaction.
7.2. $0\nu\beta\beta$ NME for $^{48}\text{Ca}$

Figure 7.3: VS-IM-SRG evolved neutrinoless double-beta decay NME of $^{48}\text{Ca}$ using a $pf$-shell valence space and the EM 1.8/2.0 interaction. For comparison, the black dashed line represents the benchmarking values from Table 7.2, using the updated $M^{0\nu}$ parameters and no SRCs. In accordance with Remark 5.1, we see that as $e_{\text{max}}$ increases, the NMEs indeed converge to a result independent of the oscillator basis frequency $\hbar\omega$. Under the sum of Equation (7.4), we can see that the Fermi and Tensor components roughly cancel, leaving the Gamow-Teller as a good approximation for the total NME, labelled as $M^{(0\nu)}$ in the top-right panel. Note that $e_{\text{max}} = 4$ results are not expected to give a consistent calculation for the $pf$-shell, hence the apparent convergence irregularities. Only two basis frequencies were available for this interaction.
Figure 7.4: VS-IM-SRG evolved neutrinoless double-beta decay NME of $^{48}$Ca using a $pf$-shell valence space and the EM 1.8/2.0 interaction, including AV18 short-range correlations. For comparison, the black dashed lines represent the benchmarking values from Table 7.2, using the updated $M^{0\nu}$ parameters, both with SRCs set to none and AV18. We also plot the $e_{\text{max}} = 10$ values from Figure 7.3 (results without SRCs) in dashed lines, with the colours corresponding to their respective $\hbar\omega$. In accordance with Remark 5.1, we see that as $e_{\text{max}}$ increases, the NMEs indeed converge to a result independent of the oscillator basis frequency $\hbar\omega$. Under the sum of Equation (7.4), we can see that the Fermi and Tensor components roughly cancel, leaving the Gamow-Teller as a good approximation for the total NME, labelled as $M^{(0\nu)}$ in the top-right panel. Note that $e_{\text{max}} = 4$ results are not expected to give a consistent calculation for the $pf$-shell, hence the apparent convergence irregularities. Only two basis frequencies were available for this interaction.
Figure 7.5: VS-IM-SRG evolved neutrinoless double-beta decay NME of $^{48}$Ca using a $pf$-shell valence space and the 500/400 $N^3$LO+3N interaction. For comparison, the black dashed line represents the benchmarking values from Table 7.2, using the updated $M^0\nu$ parameters and no SRCs. In accordance with Remark 5.1, we see that as $e_{\text{max}}$ increases, the NMEs indeed converge to a result independent of the oscillator basis frequency $\hbar \omega$. Under the sum of Equation (7.4), we can see that the Fermi and Tensor components roughly cancel, leaving the Gamow-Teller as a good approximation for the total NME, labelled as $M^{(0\nu)}$ in the top-right panel. Note that $e_{\text{max}} = 4$ results are not expected to give a consistent calculation for the $pf$-shell, hence the apparent convergence irregularities. Four basis frequencies were available for this interaction, making the convergence clearer - however, the EM 1.8/2.0 results from Figure 7.3 are considered more trustworthy, as discussed in the text.
Chapter 8

Conclusions

Modern nuclear many-body methods, such as the VS-IM-SRG using $\chi$EFT interactions, have been developed beyond simply an “innovative” status - that is, they are now an indispensable tool for calculating nuclear properties and decays. In this dissertation, we have demonstrated that VS-IM-SRG is capable of modelling rare decays, like two-neutrino double-beta decay, and exotic ones, like neutrinoless double-beta decay. What’s more is that this non-perturbative ab initio approach can capture three-body physics using two-body machinery, which is imperative for making predictions in medium mass nuclei like Calcium-48.

We report evolved NMEs for $2\nu\beta\beta$ which are roughly 3 times smaller than the phenomenological NMEs, without quenching [71, 73]. This $2\nu\beta\beta$ NME for $^{48}$Ca from VS-IM-SRG is 23% lower than the experimentally expected value, which is the opposite direction to quenching (see Figure 7.2). The inclusion of meson exchange currents did not fix this issue, and instead lowered the NME further. This is to be expected, since the $2\nu\beta\beta$ case does not use the closure approximation, and important intermediate $1^+$ states are likely missing from the $pf$-shell valence space. A comparison will be made against Coupled-Cluster theory in the near future.

Our $0\nu\beta\beta$ NMEs were approximately 20% smaller compared to ShM calculations using the GXPF1A interaction [118]. By Equation (3.18), this represents a 60% increase in the hypothetical $0\nu\beta\beta$ half-life. The inclusion of the AV18 SRC parameterization dropped $M^{0\nu}$ another 20%* - a larger difference than the 5% change seen in the phenomenological values. The primary interaction of choice in this dissertation was the EM 1.8/2.0 from $\chi$EFT [38], although more options should be studied in the future, in order to understand which interactions are most suitable for the double-beta decay operator structures (see Section 7.1 and Chapter 4).

We propose that ab initio many-body contributions are the main source of our unique NMEs. However, more research is needed to establish that this is indeed the case, as opposed to spurious CoM contamination [137] or generator cancellations (see Equation (5.10) in Section 5.2.2). A study directed at how perturbations to the closure energy alter the VS-IM-SRG evolved $0\nu\beta\beta$ NMEs is recommended. Also, since SRCs come in many different types (see Table 4.1), it would be ideal to find the optimal parameterization. A more pressing matter is running the IM-SRG evolution to higher $e_{\text{max}} = 12$ and 14, which can be done now the the new “Oak” cluster† has become available to the TRIUMF Theory Department. Upcoming studies will perform similar calculations for heavier nuclei‡ and add in ab initio theoretical uncertainties.

---

* relative to the IM-SRG evolved NMEs without any SRCs
† maintained by the UBC ARC group: https://arc.ubc.ca
‡ in particular, $^{76}$Ge and $^{82}$Se
Bibliography


Bibliography


Bibliography


Bibliography


Appendix A

Angular Momentum Coupling

When creating a state composed of many particles, we must ask: how are our good quantum numbers coupled together? By “good” quantum numbers, we mean those which are eigenvalues of a (time-independent) Hermitian operator, $\hat{T}$, which is compatible with the Hamiltonian, $\hat{H}$, so that $\partial \hat{T}/\partial t = 0$ and $[\hat{H}, \hat{T}] = 0$. This guarantees two things: i) the Hamiltonian and $\hat{T}$ are simultaneously diagonalizable, hence they share the same complete set of eigenfunctions; and ii) the quantum numbers of $\hat{T}$ will be conserved via the Heisenberg Equation of Motion \[ \frac{d}{dt} \langle \hat{T}(t) \rangle = \frac{i}{\hbar} \langle [\hat{H}, \hat{T}(t)] \rangle + \langle \frac{\partial \hat{T}}{\partial t} \rangle \]

For example, in a non-relativistic system with a spherically symmetric central potential, the orbital angular momentum, $l$, and the intrinsic angular momentum or “spin,” $s$, will be the good quantum numbers, whereas in a relativistic system the good quantum number for the Dirac equation is (total) angular momentum, also sometimes called “spin,” $\hat{J} = \hat{L} + \hat{S}$, which gives $j$. So this begs the question, which coupling schemes are most useful for certain multiple particle systems? As a brief reminder before we approach this question: the orbital angular momentum, spin, and total angular momentum all follow the same algebraic structure $[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk}\hat{L}_k$ and, $[\hat{L}^2, \hat{L}] = 0$

where $\epsilon_{ijk}$ is the Levi-Civita symbol, and the second commutation relation guarantees that the square of the vector angular momentum operator is compatible (simultaneously diagonalizable) with each component of the angular momentum, hence they share the same eigenstates. Using ladder operators, it is an undergraduate exercise to show that the eigenvalues are

$\hat{L}_z | l m \rangle = m \hbar | l m \rangle \quad \text{for} \quad -l \leq m \leq l$

$\hat{L}^2 | l m \rangle = l(l+1)\hbar^2 | l m \rangle \quad \text{where,} \quad l \in \mathbb{N}_0$

A.1 Clebsch-Gordan Coefficients

We start by defining the well known “Clebsch-Gordan (CG) coefficients.” We’ll denote these coefficients as $(j_1 m_1 j_2 m_2 \mid j m)$, which couples the states $|j_1 m_1 \rangle$ and $|j_2 m_2 \rangle$ as $|j_1 m_1 \rangle \otimes |j_2 m_2 \rangle \rightleftharpoons |j_1 m_1, j_2 m_2 \rangle$ into $|j_1 j_2; jm \rangle$, via

$|j_1 j_2; jm \rangle = \sum_{m_1, m_2} (j_1 m_1 j_2 m_2 \mid j m) |j_1 m_1, j_2 m_2 \rangle \quad \text{(A1)}$

or visa versa
A.1. Clebsch-Gordan Coefficients

\[ |j_1 m_1, j_2 m_2\rangle = \sum_{j,m} (j_1 m_1 j_2 m_2 \mid j m) |j_1 j_2, j m\rangle \]  
\[ (A2) \]

We’ll commonly refer to the coupling \( |j_1 j_2 : j m\rangle \) as “J-scheme,” and the coupling \( |j_1 m_1, j_2 m_2\rangle \) as “M-scheme.” The CG coefficients satisfy two conditions, by definition

\[ (j_1 m_1 j_2 m_2 \mid j m) = 0 \quad \text{unless,} \]
\[ m_1 + m_2 = m \quad \text{and,} \]
\[ \Delta(j_1 j_2 : j) \]  
\[ (A3) \]

where we define the “triangle condition” in Equation (A4), denoted as \( \Delta(j_1 j_2 : j) \), via

\[ |j_1 - j_2| \leq j \leq j_1 + j_2 \]  
\[ (A5) \]

The triangle condition above encodes what is meant by “coupling” quantum numbers together. You see that \( j \) is not simply the sum of the two quantum numbers \( j_1 \) and \( j_2 \), despite the fact that we have taken \( \tilde{J} = \tilde{J}_1 + \tilde{J}_2 \) in J-scheme, which we call “jj-coupling.” Compare this with what we call “ls-coupling,” when we take \( \tilde{J} = \tilde{L} + \tilde{S} \), which obeys \( \Delta(l s : j) \). The CG coefficients also obey both “orthogonality” and “completeness,” respectively written as

\[ \sum_{m_1 m_2} (j_1 m_1 j_2 m_2 \mid j m)(j_1 m_1 j_2 m_2 \mid j' m') = \delta_{jj} \delta_{mm'} \]  
\[ (A6) \]

\[ \sum_{jm} (j_1 m_1 j_2 m_2 \mid j m)(j_1 m_1' j_2 m_2' \mid j m) = \delta_{m_1 m_1'} \delta_{m_2 m_2'} \]  
\[ (A7) \]

Now we introduce an unfortunate notation commonly used in angular momentum coupling. It’s neither a quantum mechanical operator, nor a unit vector, nor just a fancy hat. It’s called the “hat factor,” and it’s simply a common prefactor written as

\[ \hat{\jmath} \equiv \sqrt{2\jmath + 1} \]  
\[ (A8) \]

As with standard convention, we define the CG coefficients such that they are real numbers. The most general form of the CG coefficients in this convention is:

**Definition A.1: “Clebsch-Gordan Coefficient”**

The coefficients, \( (j_1 m_1 j_2 m_2 \mid j m) \), that satisfy Equation (A1) and (A2), may be defined such that \( (j_1 m_1 j_2 m_2 \mid j m) \in \mathbb{R} \) via the formula

\[ (j_1 m_1 j_2 m_2 \mid j_3 m_3) = \sum_{\llbracket k \rrbracket} \frac{(-1)^k}{k!} \hat{\jmath} \]
\[ \times \frac{1}{(j_1 + j_2 - j_3 - k)!(j_1 - m_1 - k)!(j_2 + m_2 - k)!(j_3 - j_2 + m_1 + k)!(j_3 - j_1 - m_2 + k)!} \]
\[ \times \sqrt{\prod_{k=1}^{3} \left[ \sum_{n=1}^{3} (-1)^{h_{kn}} j_n \right]!} \sqrt{\prod_{n=1}^{3} (j_n + m_n)! (j_n - m_n)!} \sqrt{\left[ \sum_{n=1}^{3} j_n \right]!} \]

where we have denoted \( \| k \| \) as running that particular sum component over \( \forall k \) such that the arguments of any factorial are non-negative for the allowed values of the \( j \)'s and \( m \)'s.

There are several identities that come from this formula that we shall make use of

\[ (j_1 m_1 j_2 m_2 \mid j m) = (-1)^{j_1 + j_2 - j} (j_2 m_2 j_1 m_1 \mid j m) \quad (A9) \]

\[ = (-1)^{j_1 + j_2 - j} (j_1, -m_1, j_2, -m_2 \mid j, -m) \quad (A10) \]

\[ = (-1)^{j_1 - m_1} \hat{J}_2^{-1} (j_1 m_1, j, -m \mid j_2, -m_2) \quad (A11) \]

\[ = (-1)^{j_1 - m_1} \hat{J}_2^{-1} (j m, j_1, -m_1 \mid j_2 m_2) \quad (A12) \]

\[ (j_1 m_1 j_2 m_2 \mid 00) = \delta_{j_1 j_2} \delta_{m_1, -m_2} (-1)^{j_1 - m_1} \hat{J}_1^{-1} \quad (A13) \]

\[ (j_1 m_1 00 \mid j_2 m_2) \doteq (00 j_1 m_1 \mid j_2 m_2) = \delta_{j_1 j_2} \delta_{m_1 m_2} \quad (A14) \]

\[ (j_1 0 j_2 0 \mid j 0) = 0 \quad \text{unless, } j_1 + j_2 + j = \text{even} \quad (A15) \]

Note that many of the equations above are derivative of each other; for instance, the identity in Equation (A14) comes from (A11) with (A13), and then the equivalence is from (A9).

**Example A.1**

Due to the fermionic nature of nucleons, we will commonly take our states and anti-symmetrize them. Let’s start with our two particle states in \( M \)-scheme, with the shorthand, \( |12\rangle \equiv |j_1 m_1, j_2 m_2\rangle \) and \( |34\rangle \equiv |j_3 m_3, j_4 m_4\rangle \). Then anti-symmetrization happens via

\[ |j_1 m_1; j_2 m_2\rangle \doteq |1; 2\rangle \doteq |12\rangle_{\mathcal{A}} \equiv \frac{1}{\sqrt{2}}(|12\rangle - |21\rangle) \quad (A16) \]

Notice the notation in the equation above, where we drop the subscript \( \mathcal{A} \), representing “anti-symmetrization,” and simply use a semicolon within the ket to denote anti-symmetrization.

To find the anti-symmetrized analog in \( J \)-scheme, all we need to do is transform between \( |j_1 m_1; j_2 m_2\rangle \rightarrow |j_1 j_2; j m\rangle \) via the CG coefficients. Using Equation (A1) with Equation (A16),

\[ |j_1 m_1; j_2 m_2\rangle \rightarrow |j_1 j_2; j m\rangle = \sum_{m_1 m_2} (j_1 m_1 j_2 m_2 \mid j m) |j_1 m_1; j_2 m_2\rangle \]

\[ = \sum_{m_1 m_2} (j_1 m_1 j_2 m_2 \mid j m) \frac{1}{\sqrt{2}}(|12\rangle - |21\rangle) \]

\[ = \frac{1}{\sqrt{2}} \left[ \sum_{m_1 m_2} (j_1 m_1 j_2 m_2 \mid j m)|12\rangle \right. \]

\[ - (-1)^{j_1 + j_2 - j} \sum_{m_1 m_2} (j_2 m_2 j_1 m_1 \mid j m)|21\rangle \]

\[ \]
\[ |j_1 j_2; jm\rangle = \frac{1}{\sqrt{2}} (|j_1 j_2; jm\rangle - (-1)^{j_1 + j_2 - j} |j_2 j_1; jm\rangle) \quad (A17) \]

where in the third line we used the identity in Equation (A9).

In this example, we want to compute the inner-product between \( |12\rangle \) and \( |34\rangle \) both for \( M\)-scheme and \( J\)-scheme. In \( M\)-scheme the anti-symmetrized inner-product is straightforward

\[
\langle 1; 2|3; 4 \rangle = \frac{1}{\sqrt{2}} \left( (|12\rangle - |21\rangle) \cdot \frac{1}{\sqrt{2}} (|34\rangle - |43\rangle) \right)
\]

\[
= \frac{1}{2} \left( \langle 12|34 \rangle - \langle 12|43 \rangle - \langle 21|34 \rangle + \langle 21|43 \rangle \right)
\]

\[
= \frac{1}{2} (\delta_{13} \delta_{24} - \delta_{14} \delta_{23})
\]

\[
\langle 1; 2|3; 4 \rangle = \delta_{13} \delta_{24} - \delta_{14} \delta_{23} \quad (A18)
\]

Note that in Equation (A18) the short hand \( \delta_{ab} \equiv \delta_{n_a n_b} \delta_{l_a l_b} \delta_{s_a s_b} \delta_{j_a j_b} \delta_{m_a m_b} \) for \( a, b = 1, 2, 3, 4 \), although we will commonly omit the \( n \)'s because it is understood. Now we can use this result to find the same inner-product in \( J\)-scheme. Let’s couple our anti-symmetric states as \( |1; 2\rangle \rightarrow |j_1 j_2; jm\rangle \) and \( |3; 4\rangle \rightarrow |j_3 j_4; j'm\rangle \), to find the inner-product

\[
\langle j_1 j_2; jm|j_3 j_4; j'm' \rangle = \sum_{m_1 m_2} \sum_{m_3 m_4} (j_1 m_1 j_2 m_2 | j m\rangle (j_3 m_3 j_4 m_4 | j'm' \rangle (\delta_{13} \cdot \delta_{24} - \delta_{14} \cdot \delta_{23})
\]

\[
= \sum_{m_3 m_4} (j_1 m_3 j_2 m_4 | j m\rangle (j_3 m_3 j_4 m_4 | j'm' \rangle \delta_{13} \delta_{24} - \delta_{14} \delta_{23})
\]

\[
- \sum_{m_3 m_4} (j_1 m_4 j_2 m_3 | j m\rangle (j_3 m_3 j_4 m_4 | j'm' \rangle \delta_{13} \delta_{24} - \delta_{14} \delta_{23})
\]

\[
= \delta_{jj'} \delta_{mm'} \delta_{13} \delta_{24} - ( - 1)^{j_3 + j_4 - j'} \delta_{jj'} \delta_{mm'} \delta_{14} \delta_{23}
\]

\[
\Rightarrow \quad \langle j_1 j_2; jm|j_3 j_4; j'm' \rangle = \delta_{jj'} \delta_{mm'} [\delta_{13} \delta_{24} - ( - 1)^{j_3 + j_4 - j'} \delta_{14} \delta_{23}]
\]

\[
= \delta_{jj'} \delta_{mm'} [\delta_{13} \delta_{24} - ( - 1)^{j_1 + j_2 - j} \delta_{14} \delta_{23}] \quad (A20)
\]

In the first line above we used Equation (A9), in the second (A6), and the equivalence in the last line we leave as a simple exercise to the reader. We'll eventually find it useful to leave the coupling notation in Equation (A20) generalized, as in

---

**A.1. Clebsch-Gordan Coefficients**
\[\langle (x_1 y_1) z_1, (x_2 y_2) z_2; z m | (x_3 y_3) z_3, (x_4 y_4) z_4; z' m' \rangle = \begin{cases} \\
\delta_{zz'} \delta_{mm'} \left[ \delta_{13} \delta_{24} - (-1)^{z_3+z_4-z'+z} \delta_{14} \delta_{23} \right] \\
\delta_{zz'} \delta_{mm'} \left[ \delta_{13} \delta_{24} - (-1)^{z_1+z_2-z'} \delta_{14} \delta_{23} \right]
\end{cases}
\]

where here we used the notation \(\delta_{ab} \equiv \delta_{n_a n_b} \delta_{x_a x_b} \delta_{y_a y_b} \delta_{z_a z_b}\), for \(a, b = 1, 2, 3, 4\).

There is much physics encoded in the above math already. For instance, in the notation of Equation (A20), let’s consider the normalization where we set \(j_1 = j_2 = j_3 = j_4 \equiv j''\), and \(j = j'\), \(m = m'\), which will give

\[\langle j'' j''; j m | j'' j''; j m \rangle = 1 - (-1)^{2j''} = \begin{cases} 2, & j \text{ even} \\
0, & j \text{ odd}
\end{cases}
\]

To get the conditions above we used the fact that an individual angular momentum is a half-integer so \(2j'' = \text{odd}\), and for the phase: odd – even = odd, and odd – odd = even. This equation reveals two important points about J-scheme:

i) our anti-symmetric states only couple to even total \(j\), which encodes the Pauli principle

ii) our anti-symmetric states are still not fully normalized

To compensate for the second point above, it is common to redefine Equation (A17) as

\[|j_1 j_2; j m\rangle \equiv \frac{1}{\sqrt{2(1 + \delta_{12})}} \left( |j_1 j_2; j m\rangle - (-1)^{j_1+j_2-j} |j_2 j_1; j m\rangle \right)
\]

however, many do this normalization a posteriori. When we employ Equation (A22), it will be made entirely explicit. Note that, in this scheme: \(|j_1 j_2; j m\rangle = |(l_1 s_1) j_1, (l_2 s_2) j_2; j m\rangle\) and \(|j_2 j_1; j m\rangle = |(l_2 s_2) j_2, (l_1 s_1) j_1; j m\rangle\). We leave it as a small exercise for the reader to check that Equation (A22) indeed yields \(|j'' j''; j m\rangle = |j'' j''; j m\rangle\) for even total \(j\).

A.2 The Wigner 3j-Symbols

In the equations of angular momentum coupling, Eugene Wigner, a pioneer of symmetries in quantum mechanics [166], must have noticed a peculiar pattern between phase factors, hat factors, and alike. Hence, the following definition was made:

**Definition A.2:** “(Wigner) 3j-Symbols”

\[
\begin{pmatrix}
  j_1 & j_2 \\
  m_1 & m_2
\end{pmatrix}
\equiv (-1)^{j_1-j_2-m} j^{-1} (j_1 m_1 j_2 m_2 | j, -m)
\]

(A23)
Physically, the $3j$-symbol is the probability amplitude that three states are coupled to produce zero angular momentum. That is

$$
\left( \begin{array}{ccc}
  j_1 & j_2 & j_3 \\
  m_1 & m_2 & m_3 \\
\end{array} \right) \propto \sum_{j_1' m_1'} (j_1 m_1 j_2 m_2 | j_1' m_1' j_2' m_2' | 0 0)
$$

Clearly the $3j$-symbol will inherit the relevant conditions in Equation (A3) and (A4) from the CG coefficient on the RHS of Equation (A23). So we’ll get the conditions

$$
\left( \begin{array}{ccc}
  j_1 & j_2 & j \\
  m_1 & m_2 & m \\
\end{array} \right) = 0 \text{ unless,}
$$

$$
m_1 + m_2 + m = 0 \text{ and,}
$$

$$
\Delta(j_1 j_2 : j) \tag{A24}
$$

It is important to note the use of parenthesized matrix notation for the Wigner $3j$-symbol itself, as the type of brackets used will distinguish it from the other Wigner symbols to come. The $3j$-symbol has the symmetry that switching any two columns will yield a phase factor, for example switching the second and third columns yields

$$
\left( \begin{array}{ccc}
  j_1 & j_2 & j \\
  m_1 & m_2 & m \\
\end{array} \right) \doteq (-1)^{-j_1 - j_2 - j} \left( \begin{array}{ccc}
  j_1 & j & j_2 \\
  m_1 & m & m_2 \\
\end{array} \right) \doteq ... \tag{A26}
$$

### A.3 Coupling Three Angular Momenta

The CG coefficients are useful for coupling two particles together between $M$-scheme and $J$-scheme. The next natural question is: how does one couple more than two particles? We start by coupling three particles, each associated with compatible $J_1, J_2,$ and $J_3,$ into $\tilde{J} = J_1 + J_2 + J_3.$ There are three intermediate ways we can couple to produce $\tilde{J}$: couple particle 1 to 2, and then the result to 3; couple 2 to 3, and then the result to 1; or couple 1 to 3, and the result to 2.

To transform between these couplings, we define the analog to CG coefficients, known as the “6$j$-symbols.” For instance:

**Definition A.3: “(Wigner) 6$j$-Symbols”**

To transform from the $jjj$-couplings $\tilde{J}_{12} = \tilde{J}_1 + \tilde{J}_2,$ $\tilde{J} = \tilde{J}_{12} + \tilde{J}_3$ to $\tilde{J}_{23} = \tilde{J}_2 + \tilde{J}_3,$ $\tilde{J} = \tilde{J}_{12} + \tilde{J}_3,$ we use the “(Wigner) 6$j$-symbol,” denote as

$$
\left( \begin{array}{ccc}
  j_1 & j_2 & j_{12} \\
  j_3 & j & j_{23} \\
\end{array} \right)
$$

in the $J$-scheme summation

$$
|j_1, (j_2 j_3) j_{23}; j m\rangle = \sum_{j_{12}} (-1)^{j_1 + j_2 + j_3 + j_{12}} \tilde{J}_{12} \tilde{J}_{23} \left( \begin{array}{ccc}
  j_1 & j_2 & j_{12} \\
  j_3 & j & j_{23} \\
\end{array} \right) |(j_1 j_2) j_{12}, j:j m\rangle
$$

It can be shown that the 6$j$-symbols are related to the 3$j$-symbols, and in turn to the CG
coefficients of two particle coupling, via the formula

\[
\begin{pmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{pmatrix} \equiv \sum_{m_1, \ldots, m_6} (-1)^{\sum_{k=1}^{6}(j_k-m_k)} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_5 & j_6 \\ -m_1 & m_5 & m_6 \end{pmatrix} \times \begin{pmatrix} j_4 & j_5 & j_3 \\ m_4 & -m_5 & m_3 \end{pmatrix} \begin{pmatrix} j_4 & j_2 & j_6 \\ -m_4 & -m_2 & -m_6 \end{pmatrix}
\]

and that they must obey the triangle conditions

\[
\begin{pmatrix} J_1 & J_2 & J_3 \\ j_1 & j_2 & j_3 \end{pmatrix} = 0 \quad \text{unless,} \quad \begin{cases} \Delta(J_1 J_2 : J_3), \Delta(j_1 j_2 : j_3) \\ \Delta(J_1 J_2 : j_3), \Delta(J_1 j_2 : j_3) \end{cases}
\] (A27)

Similar to Equation (A26) for 3j-symbols, the 6j-symbols will be invariant under a swap of any two columns horizontally, or the vertical reflection of any two columns as so

\[
\begin{pmatrix} J_1 & J_2 & J_3 \\ j_1 & j_2 & j_3 \end{pmatrix} = \begin{pmatrix} J_1 & J_3 & J_2 \\ j_1 & j_3 & j_2 \end{pmatrix} = \begin{pmatrix} J_3 & J_2 & J_1 \\ j_3 & j_2 & j_1 \end{pmatrix} = \ldots
\] (A28)

\[
\begin{pmatrix} J_1 & J_2 & J_3 \\ j_1 & j_2 & j_3 \end{pmatrix} = \begin{pmatrix} J_1 & J_2 & J_3 \\ j_1 & j_2 & j_3 \end{pmatrix} = \begin{pmatrix} J_1 & J_2 & J_3 \\ j_1 & j_2 & j_3 \end{pmatrix} = \ldots
\] (A29)

Finally, if the lower right entry of the 6j-symbol is zero, we can reduce the 6j-symbol as follows

\[
\begin{pmatrix} J_1 & J_2 & J_3 \\ j_1 & j_2 & 0 \end{pmatrix} = \delta_{(j_1 j_2 : j_3)} \delta_{j_1 j_2} \delta_{j_2 j_3} (-1)^{j_1+j_2+j_3} \hat{J}_1^{-1} \hat{J}_2^{-1}
\] (A30)

where we’ve introduced the so-called “triangular delta,” defined by

\[
\delta_{(j_1 j_2 : j)} \equiv \begin{cases} 1, & \Delta(j_1 j_2 : j) \\ 0, & \text{o.w.} \end{cases}
\] (A31)

### A.4 Coupling Four Angular Momenta

The coupling coefficients for four particles are known as “normalized 9j-symbols.” Unlike the 6j-symbols, these are denoted by square brackets:

**Definition A.4: “(Wigner) 9j-Symbols”**

To transform from the $jj$-couplings $\hat{J}_{12} = \hat{J}_1 + \hat{J}_2$, $\hat{J}_{34} = \hat{J}_3 + \hat{J}_4$, $\hat{J} = \hat{J}_{12} + \hat{J}_{34}$ to $\hat{J}_{13} = \hat{J}_1 + \hat{J}_3$, $\hat{J}_{24} = \hat{J}_2 + \hat{J}_4$, $\hat{J} = \hat{J}_{13} + \hat{J}_{24}$, we use the “normalized (Wigner) 6j-symbol”

\[
\begin{pmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{pmatrix}
\]

in the $J$-scheme summation

\[
|\{j_1 j_3\} j_{13}, (j_2 j_4) j_{24} : j m\} = \sum_{j_{12} j_{34}} |\{j_1 j_2\} j_{12}, (j_3 j_4) j_{34} : j m\} |\{j_{12} j_{34}\} j_{12} j_{34} : j m\} \quad \text{(A32)}
\]
A.4. Coupling Four Angular Momenta

The standard "(Wigner) 9j-symbols" are denoted by curly brackets, and are related to the normalized 9j-symbol simply by a product of hat factors

\[
\begin{pmatrix}
  j_1 & j_2 & j_{12} \\
  j_3 & j_4 & j_{34} \\
  j_{13} & j_{24} & j
\end{pmatrix}
\equiv \hat{j}_{12}\hat{j}_{34}\hat{j}_{13}\hat{j}_{14}
\begin{pmatrix}
  j_1 & j_2 & j_{12} \\
  j_3 & j_4 & j_{34} \\
  j_{13} & j_{24} & j
\end{pmatrix}
\]  

(A33)

By construction, the normalized Wigner 9j-symbols can also be used to transform from ls-coupling to jj-coupling, simply by relabelling Equation (A32) as

\[
|l_1s_1j_1, l_2s_2j_2: jm\rangle = \sum_{l,s} \begin{pmatrix}
  l_1 & l_2 & l \\
  s_1 & s_2 & s \\
  j_1 & j_2 & j
\end{pmatrix}
|l_1l_2j_1, l_2s_2j_2: jm\rangle
\]  

(A34)

It can be shown that the 9j-symbols are related to the 3j-symbols, and in turn to the 6j-symbols of three particle coupling, via the mnemonic "rap one byt, rob any pet" as follows

\[
\begin{pmatrix}
  r & a & p \\
  o & n & e \\
  b & y & t
\end{pmatrix}
= \sum_{m' s} \begin{pmatrix}
  r & a & p \\
  m_r & m_a & m_p \\
  o & n & e \\
  m_o & m_n & m_e \\
  b & y & t \\
  m_b & m_y & m_t
\end{pmatrix}
\times \begin{pmatrix}
  r & o & b \\
  m_r & m_o & m_b \\
  a & n & y \\
  m_a & m_n & m_y \\
  p & e & t \\
  m_p & m_e & m_t
\end{pmatrix}
\]  

\[
\sum_M (-1)^{2M} \begin{pmatrix}
  r & o & b \\
  y & t & M \\
  a & n & e \\
  M & e & M \\
  p & e & t \\
  M & r & a
\end{pmatrix}
\]  

(A35)

and that they must obey the triangle conditions for each of their rows and columns

\[
\begin{pmatrix}
  r & a & p \\
  o & n & e \\
  b & y & t
\end{pmatrix} = 0 \text{ unless } \left\{ \begin{array}{l}
\Delta(r o:b), \Delta(a n:y), \Delta(p e:t) \\
\Delta(r a:p), \Delta(o n:e), \Delta(b y:t)
\end{array} \right.
\]  

(A37)

A particularly useful identity of the 9j-symbol is that by switching any two rows or columns, we pick up a phase factor of the sum of the components, \( \Sigma \equiv r + o + b + a + n + y + p + e + t \). For example, we can switch the first and third rows, or the first and third columns, via

\[
\begin{pmatrix}
  r & a & p \\
  o & n & e \\
  b & y & t
\end{pmatrix} \overset{\Sigma}{\rightarrow} (-1)^\Sigma \begin{pmatrix}
  b & y & t \\
  o & n & e \\
  r & a & p
\end{pmatrix} \overset{\Sigma}{\rightarrow} (-1)^\Sigma \begin{pmatrix}
  p & a & r \\
  e & n & o \\
  t & y & b
\end{pmatrix} \overset{\Sigma}{\rightarrow} ...
\]  

(A38)

Finally, a 9j-symbol with a zero entry can be reduced down to a 6j-symbol, as follows

\[
\begin{pmatrix}
  j & u & R \\
  l & c & r \\
  D & d & 0
\end{pmatrix} \overset{\Sigma}{\rightarrow} \delta_{Rr} \delta_{Dd} (-1)^{u+R+l+D} \begin{pmatrix}
  j & u & R \\
  l & c & l \\
  D & d & D
\end{pmatrix}
\]  

(A39)

A nice here trick is: if any other arbitrary element of a 9j-symbol is zero, then by repeatedly using Equation (A38) and then (A39), such a 9j-symbol can be reduced to a 6j-symbol.
Appendix B

Spherical Tensor Operators

In quantum mechanics, we need a meaningful definition of “tensors,” in conjunction with any other field. Tensors in physics are defined by their ability to transform in a manner that encodes the geometry of said physical system. In fluid mechanics, one uses tensors that transform in a Cartesian space; they rotate in the three dimensions of Euclidean geometry. In General Relativity, one uses tensors that transform in a spacetime; they hyper-rotate in a locally Lorentzian manifold of four dimensional Riemannian geometry. The case is wildly different in quantum mechanics, since our geometrical structure is encoded by the coupling of angular momenta.

B.1 Definitions

Consider a rotation, $R \in \text{SO}(3)$, which may be parameterized by Euler angles or rotations about the $x, y, z$ axes, etc. In quantum mechanics, the unitary form of $R$ is generated by the angular momentum operator. That is, for the rotation about $\hat{n}$ by the angle $\theta$, then

$$U(R(\theta)) = \exp(-i\theta \hat{L}/\hbar) \in \text{SU}(2) \quad \text{(B1)}$$

We can encapsulate how these unitary rotations transform quantum states by making the following definition:

Definition B.1: “Wigner D-Matrix”

For a unitary rotation, such as the one in Equation (B1) above, acting on the state $|lm\rangle$, the “Wigner D-Matrix” is defined by

$$D_{lm'm}^l \equiv \langle lm'|U(R)|lm\rangle = \sum_{m'} D_{lm'm}^l |lm'\rangle \quad \text{(B2)}$$

Now that we have a way of rotating states, we can define a “spherical tensor (operator)” as an operator which transforms under rotations as so:

Definition B.2: “Spherical Tensor (Operator)”

If an operator, labelled $\hat{T}_{LM}$, transforms under a unitary rotation, such as the one in Equation (B1), via the Wigner D-Matrix like

$$U(R)\hat{T}_{LM}U^\dagger(R) = \sum_{M'} D_{M'M}^L \hat{T}_{LM'}$$
then it is said to be a “spherical tensor (operator)” of rank $L$. It is called “spherical” since the indices will obey the same algebraic structure as spherical harmonics

$$M = -L, -L + 1, ... , L - 1, L$$

Since the range of $M$ is determined by the value of $L$, it is common to make the shorthand $\tilde{T}_{LM} \rightarrow \tilde{T}_L$. Spherical tensors with $L = 0$ or 1 will often be referred to as “scalar” or “vector” operators, respectively.

You might be wondering about how to construct products of spherical tensor operators. Unfortunately, our typical matrix multiplication does not necessarily produce a spherical tensor! Symbolically, if $\mathcal{ST}$ represents the space of all spherical tensor operators, we want to formulate a tensor product such that $[\cdot \otimes \cdot] : \mathcal{ST} \times \mathcal{ST} \rightarrow \mathcal{ST}$. Since CG coefficients encode angular momentum, the most intuitive move is to insert them within the matrix multiplication:

**Definition B.3: “(Spherical) Tensor Product”**

Consider two spherical tensor operators, denoted $\hat{A}_{L_1}$ and $\hat{B}_{L_2}$, then the “(spherical) tensor product” between these two spherical tensors is defined as

$$\hat{T}_{LM} = [\hat{A}_{L_1} \otimes \hat{B}_{L_2}]_{LM} \equiv \sum_{M_1, M_2} (L_1 M_1 L_2 M_2 | L M) \hat{A}_{L_1 M_1} \hat{B}_{L_2 M_2}$$

(B3)

**Remark B.1**

The tensor product $\hat{T}_{LM}$, as defined in Definition B.3, is indeed a spherical tensor of rank $L$, where $L$ obeys the triangle condition $\Delta(L_1 L_2 : L)$.

Let’s go over an important example with the definition of the tensor product - a spherical tensor product with the identity. Our intuition says that this tensor product should return the original tensor itself, especially if this product forms some kind of monoid or group structure on the set of all spherical tensors.

**Example B.1**

We note that the identity operator, $\hat{1}$, is a scalar spherical tensor operator, hence its $M$ values only run over $M = 0$, i.e. $\hat{1} \equiv \hat{1}_0 = \hat{1}_{00}$. So, taking the tensor product of $\hat{1}_{00}$ with an arbitrary spherical tensor, $\hat{T}_{LM'}$, will give a spherical tensor of rank $R$, where we have $\Delta(0 L : R) \Rightarrow R = L$. And so Equation (B3) gives us

$$[\hat{1}_{00} \otimes \hat{T}_L]_{LM} = \sum_{M'} (00 L M' | L M) \hat{T}_{LM'} = \sum_{M'} \delta_{M'M} \hat{T}_{LM} = \hat{T}_{LM}$$

$$\Rightarrow \hat{T}_{LM} = [\hat{1}_0 \otimes \hat{T}_L]_{LM}$$

where, in the second step of the first line, we used Equation (A14). Repeating similar math
will give \( \hat{T}_{LM} = [\hat{T}_L \otimes \mathbb{1}_0]_{LM} \) as well, hence
\[
\hat{T}_{LM} = [\mathbb{1}_0 \otimes \hat{T}_L]_{LM} = [\hat{T}_L \otimes \mathbb{1}_0]_{LM}
\] (B4)

In other words, the identity, as a spherical tensor operator of rank \( L = 0 \), gives us the identity element under the spherical tensor product operation.

A common scenario in many-body quantum mechanics is the need to take tensor products of tensor products. Many of these types of formulae can be found in Section 3.3 of [15]. Before we present one of these, we must make another definition:

**Definition B.4: “Commutation Under the Tensor Product”**

Consider the “commutator of a tensor product” between the spherical tensors \( \hat{A}_{L_1} \) and \( \hat{B}_{L_2} \)
\[
[\hat{A}_{L_1}, \hat{B}_{L_2}]_{LM} \equiv \hat{A}_{L_1} \otimes \hat{B}_{L_2} \otimes \mathbb{1}_0 - (-1)^{L_1+L_2-L} \hat{B}_{L_2} \otimes \hat{A}_{L_1} \otimes \mathbb{1}_0
\] (B5)

which is, itself, a spherical tensor operator of rank \( L \). Then, when \( [\hat{A}_{L_1}, \hat{B}_{L_2}]_{LM} = 0 \) the spherical tensors \( \hat{A}_{L_1} \) and \( \hat{B}_{L_2} \) are said to “commute under the tensor product.” The phase in front of the second term on the RHS of Equation (B5) comes from the identity in Equation (A9) used within Definition B.3.

For the spherical tensors \( \hat{A}_{L_1}, \hat{B}_{L_2}, \hat{C}_{L_3}, \hat{D}_{L_4} \), which may not necessarily commute under the tensor product, Equation (20) in Section 3.3.3 of [15] gives the tensor recoupling formula
\[
[\hat{A}_{L_1} \otimes \hat{B}_{L_2}]_{L_12} \otimes [\hat{C}_{L_3} \otimes \hat{D}_{L_4}]_{L_34} =
\sum_{L_13L_24} \left[ \begin{array}{ccc} L_1 & L_2 & L_{12} \\ L_3 & L_4 & L_{34} \\ L_{13} & L_{24} & L \\
\end{array} \right] \left[ \begin{array}{ccc} \hat{A}_{L_1} \otimes \hat{C}_{L_3} & [\hat{B}_{L_2} \otimes \hat{D}_{L_4}]_{L_24} \\ \end{array} \right]_{LM}
\]
\[
+ \sum_{RS} \left( (-1)^{L_1+L_3+L_4-L_{34}-L-R} \hat{L}_1 \hat{L}_3 \hat{R} \hat{S} \left\{ \begin{array}{ccc} L_1 & L_2 & L_{12} \\ L_{34} & L & R \\
\end{array} \right\} \right) \left\{ \begin{array}{ccc} L_3 & L_4 & L_{34} \\ R & L_2 & S \\
\end{array} \right\}
\times \left[ \hat{A}_{L_1} \otimes [\hat{B}_{L_2} \otimes \hat{C}_{L_3} \otimes \hat{D}_{L_4}]_{S,R} \right]_{LM}
\] (B6)

where we’ve used Equation (B5) between \( \hat{B}_{L_2} \) and \( \hat{C}_{L_3} \) in the bottom line. Finally, we may define the notion of a scalar product within the spherical tensor framework:

**Definition B.5: “(Spherical Tensor) Scalar Product”**

Consider two spherical tensors, \( \hat{T} \) and \( \hat{S} \), both of rank \( L \). Then we define their “(spherical tensor) scalar product” as a rank 0 spherical tensor operator via
\[
\hat{T}_L \otimes \hat{S}_L \equiv (-1)^L \hat{L} \left[ \hat{T}_L \otimes \hat{S}_L \right]_{00} = \sum_M (-1)^M \hat{T}_{LM} \hat{S}_{L,-M}
\] (B7)

The equivalence above can be shown easily by applying Equation (B3), then using Equa-
B.2 Reduced Matrix Elements

In nuclear physics, it will often be useful to (in some sense) “integrate out” the projected quantum numbers of our nuclear states. Consider the two states $|j m\rangle$ and $|j' m'\rangle$, each with their own corresponding wave-functions, $\psi_{j m}(\vec{r})$ and $\psi_{j' m'}(\vec{r})$, respectively. These wave-functions could describe scalar particles, vector particles, or even tensor particles, and hence they may be thought of as tensor operators, in the sense of quantum field theory. We may then make a seemingly random definition, which we take from [167]:

Definition B.6: “Reduced Matrix Elements”

For the states $|j m\rangle$ and $|j' m'\rangle$, the “reduced matrix elements” of a spherical tensor operator, $\hat{T}_L$, are defined by

$$\langle j | \hat{T}_L | j' \rangle \equiv ((-1)^{j-L+j'} \int d\tau [\bar{\varphi}_j \otimes [\hat{T}_L \otimes \bar{\psi}_{j'}]_0]_0$$

where the modified wave-function $\bar{\varphi}_{j m} \equiv (-1)^{j+m} \psi_{j,-m}$, and the wave-functions are treated as spherical tensor operators of rank $j$ and $j'$ respectively.

Definition B.6 gives us a way of writing matrix elements that do not explicitly depend on the projected quantum numbers $m$ and $m'$. The existence of these so-called reduced matrix elements is critical to developing nuclear structure theory within the context of many-body quantum mechanics. So the next natural question is: how do we relate them to what we already know how to calculate?

B.3 The Wigner-Eckart Theorem

We are now ready to introduce the first theorem relevant to the work presented in this dissertation. We will state it without proof, but much deeper insight can be provided in the context of nuclear theory by [167]. In the context of group theory, and the relationship between Lie algebras and angular momentum quantization representations via coupling coefficients, mathematically rigorous proofs can be found in [168, 169]. Without further ado:

Theorem B.1: “The Wigner-Eckart Theorem”

For a spherical tensor operator $\hat{T}$, of rank $L$, with the set of quantum numbers $\eta'$ and $\eta$ additional to those listed below, the matrix elements of $\hat{T}$ will be related to the reduced matrix elements by a phase and a $3j$-symbol, as follows:

$$(\hat{T}_{L+\eta',\eta})_{j, j'} = ((-1)^{j-L+j'} \int d\tau [\bar{\varphi}_j \otimes [\hat{T}_L \otimes \bar{\psi}_{j'}]_0]_0)$$
B.3. The Wigner-Eckart Theorem

\[ \langle \eta j m | T_{LM} | \eta' j' m' \rangle = \gamma^{-1}(j' m' L M | j m) \langle \eta j | T_L | \eta' j' \rangle \]  \hspace{1cm} (B8)

\[ \doteq ( -1)^{j - m} \left( \begin{array}{cc} j & j' \\ L & M \end{array} \right) \langle \eta j | T_L | \eta' j' \rangle \]  \hspace{1cm} (B9)

This is, quite simply, a stunning and highly useful theorem! In essence, what it says is that the coupling coefficients that we’ve developed can fully encode the decoupling of full matrix elements into their respective reduced matrix elements. Thus, through Theorem B.1, we have a means to convert between the matrix element scheme of our choice. If we can calculate the reduced matrix elements, then we don’t have to carry projected quantum numbers until they are needed. Practically speaking, this will significantly reduce the amount of calculations required for certain computations. All that is needed now, is a means of calculating the reduced elements themselves. First, we work through a couple simple examples:

**Example B.2**

We derive Equation (2.33) in [5], by noticing Equation (B8) with the rank \( L = 0 \) identity operator, and dropping the additional quantum numbers \( \eta, \eta' \), gives

\[ \langle j m | 1 | j' m' \rangle = \delta_{jj'} \delta_{mm'} = \gamma^{-1}(j' m' 0 M | j m) \langle j | 1 | j' \rangle \]  \hspace{1cm} (B10)

The CG coefficient on the RHS has to obey the condition in Equation (A3), or else Equation (B10) above will be trivial. Hence, since it must be that \( m = m' \) via the Kronecker-delta on the LHS, we have: \( m' + M = m = m' \Rightarrow M = 0 \). Equation (B10) becomes

\[ \delta_{jj'} \gamma = (j' m' 0 0 | j m) \langle j | 1 | j' \rangle \]

For \( j \neq j' \) clearly we get \( \langle j | 1 | j' \rangle = 0 \), and for \( j = j' \) we may use Equation (A14) to obtain the useful reduced matrix elements

\[ \langle j | 1 | j' \rangle = \delta_{jj'} \gamma \]  \hspace{1cm} (B11)

Notice that, had we used the quantum number \( l \) in replace of \( j \), we can more explicitly write:

\[ \langle n l m | 1 | n' l' m' \rangle = \delta_{nn'} \delta_{ll'} \delta_{mm'} \]  in Equation (B10). Hence, we’d need to carry the additional quantum number \( \eta = n \) in the Wigner-Eckart Theorem, which would give

\[ \langle n l | 1 | n' l' \rangle = \delta_{nn'} \delta_{ll'} \gamma \]  \hspace{1cm} or, equivalently \hspace{1cm} (B12)

\[ \langle l | 1 | l' \rangle = \delta_{ll'} \gamma \]

The second line above is a common abuse of notation, where we will omit writing the \( n \)’s, even though they should certainly be included computationally.
Example B.3
Another operator that often comes up within reduced matrix elements are the “spherical tensor harmonics.” These are simply the analog of spherical harmonics, $Y_{LM}$ as in Equation (F7), treated as a spherical tensor operator, $\hat{Y}_L$. The reduced matrix elements of a spherical tensor harmonic of rank $L$ are presented in Equation (F8). In this example, we’ll calculate the reduced matrix elements of $\hat{Y}_L$ augmented by some arbitrary, well-behaved function, $f(r)$. We start with the non-reduced matrix elements for one-body states

$$
\langle n l m | f(r) Y_{LM}(\vec{r}) | n' l' m' \rangle = \int dr r^2 \int d\Omega \, \psi^*_{nlm}(\vec{r}) f(r) Y_{LM}(\vec{r}) \psi_{n'l'm'}(\vec{r})
$$

$$
= \int dr r^2 R^*_{nl}(r) f(r) R_{n'l'}(r) \int d\Omega \, Y^*_{lm}(\theta, \phi) Y_{LM}(\vec{r}) Y_{l'm'}(\theta, \phi)
$$

$$
\Rightarrow \langle n l || f(r) \hat{Y}_L(\vec{r}) || n' l' \rangle = \langle n l || f(r) || n' l' || \hat{Y}_L || l' \rangle \quad (B13)
$$

where we separated the variables of the wave-functions as: $\psi_{nlm}(\vec{r}) = R_{nl}(r)Y_{lm}(\theta, \phi)$, in accordance with the TISE and the definition of spherical harmonics. Inserting Equation (F8) into (B13) with (A23) and $l, L \in \mathbb{N}_0$ gives

$$
\langle n l || f(r) \hat{Y}_L(\vec{r}) || n' l' \rangle = \frac{(-1)^L \sqrt{L}}{\sqrt{4\pi}} \langle l 0 L 0 || l' 0 \rangle \langle n l || f(r) || n' l' \rangle \quad (B14)
$$

noting that Equation (B14) is 0 unless $l + L + l' = \text{even}$, by the identity in Equation (A15).

B.4 Decomposition Theorems

We’ll now put forth several theorems which expand the calculation tools for reduced matrix elements. The first of these “decomposition” theorems that we list is:

**Theorem B.2**
Consider the spherical tensor product made up of the spherical tensors $\hat{A}_L_1$ and $\hat{B}_L_2$ by

$$
\hat{T}_{LM} \equiv [\hat{A}_{L_1} \otimes \hat{B}_{L_2}]_{LM}
$$

then, given that $\hat{J}_1$ and $\hat{J}_2$ commute and likewise for the primed versions, the symmetrized $J$-scheme reduced matrix elements of the tensor product and its component tensors obey

$$
\langle j_1 j_2 : j || \hat{T}_L || j'_1 j'_2 : j' \rangle = \hat{\gamma} \hat{\gamma}' \left\{ \begin{array}{ccc}
\frac{1}{2} & j_1 & j_2 \\
\frac{1}{2} & j'_1 & j'_2 \\
L_1 & L_2 & L
\end{array} \right\} \langle j_1 || \hat{A}_{L_1} || j'_1 \rangle \langle j_2 || \hat{B}_{L_2} || j'_2 \rangle \quad (B15)
$$

One issue to point out is that since $\hat{T}_{LM}$ is, by construction, a two-body operator, the matrix elements can either be symmetrized or anti-symmetrized, depending on how the states are
set. For a fermionic system we would prefer the latter, so it’s important to take note that Equation (B15) is the symmetrized version. To take care of this issue and anti-symmetrize, see Theorem B.4 below. Theorem B.2 leads to a few useful corollaries:

**Corollary B.2.1**

Consider two spherical tensors, $\hat{T}$ and $\hat{S}$, both of rank $L$. We can relate the symmetrized $J$-scheme reduced matrix elements of their scalar product by

$$\langle j_1 j_2; j | \hat{T}_{L} \hat{S}_L | j'_1 j'_2; j' \rangle = \delta_{jj'} (-1)^{j_2+j+1} \hat{J} \hat{L} \hat{J}^{-1} \hat{L}^{-1} \delta_{LL} \delta_{JJ} (-1)^{j_2+j+j'_1+j'+L} \hat{J} \hat{L} \hat{J}^{-1} \hat{L}^{-1} \langle j_1 | \hat{T}_L | j'_1 \rangle \langle j_2 | \hat{S}_L | j'_2 \rangle$$

Equation (B15) now gives

$$\langle j_1 j_2; j | \hat{T}_{L} \hat{S}_L | j'_1 j'_2; j' \rangle = (-1)^L \hat{L} \hat{J} \hat{L} \hat{J}^{-1} \delta_{LL} \delta_{JJ} (-1)^{j_2+j+j'_1+j'+2L} \hat{J} \hat{L} \hat{J}^{-1} \hat{L}^{-1} \langle j_1 | \hat{T}_L | j'_1 \rangle \langle j_2 | \hat{S}_L | j'_2 \rangle$$

Equation (B17) now gives

$$\langle j_1 j_2; j | \hat{T}_{L} \hat{S}_L | j'_1 j'_2; j' \rangle = (-1)^L \hat{L} \hat{J} \hat{L} \hat{J}^{-1} \delta_{LL} \delta_{JJ} (-1)^{j_2+j+j'_1+j'+2L} \hat{J} \hat{L} \hat{J}^{-1} \hat{L}^{-1} \langle j_1 | \hat{T}_L | j'_1 \rangle \langle j_2 | \hat{S}_L | j'_2 \rangle$$

We can reduce Equation (B17) by noticing that $\hat{0} = 1$, and Equation (A39) yields

$$\langle j_1 j_2; j | \hat{T}_{L} \hat{S}_L | j'_1 j'_2; j' \rangle = \delta_{JJ} \delta_{LL} (-1)^{j_2+j+j'_1+j'+2L} \hat{J} \hat{L} \hat{J}^{-1} \hat{L}^{-1} \langle j_1 | \hat{T}_L | j'_1 \rangle \langle j_2 | \hat{S}_L | j'_2 \rangle$$

**Proof of Corollary (B.2.1).**

We begin by plugging Equation (B7) into the structure of Theorem B.2, hence

$$\langle j_1 j_2; j | \hat{T}_{L} \hat{S}_L | j'_1 j'_2; j' \rangle = \delta_{jj'} (-1)^{j_2+j+1} \hat{J} \hat{L} \hat{J}^{-1} \hat{L}^{-1} \delta_{LL} \delta_{JJ} (-1)^{j_2+j+j'_1+j'+2L} \hat{J} \hat{L} \hat{J}^{-1} \hat{L}^{-1} \langle j_1 | \hat{T}_L | j'_1 \rangle \langle j_2 | \hat{S}_L | j'_2 \rangle$$

Equation (B15) now gives

$$\langle j_1 j_2; j | \hat{T}_{L} \hat{S}_L | j'_1 j'_2; j' \rangle = (-1)^L \hat{L} \hat{J} \hat{L} \hat{J}^{-1} \delta_{LL} \delta_{JJ} (-1)^{j_2+j+j'_1+j'+2L} \hat{J} \hat{L} \hat{J}^{-1} \hat{L}^{-1} \langle j_1 | \hat{T}_L | j'_1 \rangle \langle j_2 | \hat{S}_L | j'_2 \rangle$$

We can reduce Equation (B17) by noticing that $\hat{0} = 1$, and Equation (A39) yields

$$\langle j_1 j_2; j | \hat{T}_{L} \hat{S}_L | j'_1 j'_2; j' \rangle = \delta_{JJ} \delta_{LL} (-1)^{j_2+j+j'_1+j'+2L} \hat{J} \hat{L} \hat{J}^{-1} \hat{L}^{-1} \langle j_1 | \hat{T}_L | j'_1 \rangle \langle j_2 | \hat{S}_L | j'_2 \rangle$$

Clearly $\delta_{LL} = 1$ and subbing Equation (B18) into (B17) will cancel the hat factors $\hat{L}$ and $\hat{J}$

$$\langle j_1 j_2; j | \hat{T}_{L} \hat{S}_L | j'_1 j'_2; j' \rangle = \delta_{JJ} \delta_{LL} (-1)^{j_2+j+j'_1+j'+2L} \hat{J} \hat{L} \hat{J}^{-1} \hat{L}^{-1} \langle j_1 | \hat{T}_L | j'_1 \rangle \langle j_2 | \hat{S}_L | j'_2 \rangle$$

By the $\delta_{JJ}$ above, we have that $j = j' \rightarrow j' = j$. Also, since $L \in \mathbb{N}_0 \rightarrow 2L = \text{even} \forall L$, therefore $(-1)^{2L} = +1$. Putting all this into Equation (B19) retrieves (B16).

□

**Corollary B.2.2**

Consider two spherical tensors, $\hat{T}$ and $\hat{S}$, both of rank 0. We note that their tensor product is equivalent to their scalar product, since by Equation (B7) we have

$$\hat{T}_{0} \hat{S}_0 = (-1)^0 \hat{T}_0 \otimes \hat{S}_0 = \hat{T}_0 \otimes \hat{S}_0$$

109
We can then relate the symmetrized matrix elements of their scalar tensor product by
\[
\langle j_1 j_2; j | \hat{T}_0 \circ \hat{S}_0 | j'_1 j'_2; j' \rangle = \delta_{j_1 j_2} \delta_{j_1 j'_1} \delta_{j_2 j'_2} \tilde{\gamma}^{j j' j'_{2 1}} \langle j_1 | \hat{T}_0 | j'_1 \rangle \langle j_2 | \hat{S}_0 | j'_2 \rangle \tag{B21}
\]

Note that in the literature the Kronecker-deltas and the triangular delta might be understood, and so Equation (B21) can be written more compactly as
\[
\langle j_1 j_2; j | \hat{T}_0 \circ \hat{S}_0 | j_1 j_2; j \rangle = \frac{\tilde{\gamma}^{j j' j'_{2 1}}}{j_1 j_2} \langle j_1 | \hat{T}_0 | j_1 \rangle \langle j_2 | \hat{S}_0 | j_2 \rangle
\]
However, for purposes of clarity, we will rarely use this convention, unless explicitly stated.

**Proof of Corollary (B.2.2).**

This is an extension of Corollary B.2.1 above, so we simply use Equation (B16) to get
\[
\langle j_1 j_2; j | \hat{T}_0 \circ \hat{S}_0 | j'_1 j'_2; j' \rangle = \delta_{j_1 j'_1} \delta_{j_2 j'_2} \delta_{j j' j_{2 1}} \langle j_1 | \hat{T}_0 | j'_1 \rangle \langle j_2 | \hat{S}_0 | j'_2 \rangle \tag{B22}
\]
Within this equation, we see that we can apply the 6j-symbol identity in Equation (A30), so
\[
\begin{pmatrix} j_1 & j_2 & j \\ j'_1 & j'_2 & j' \end{pmatrix} = \delta_{(j_1,j_2;j')} \delta_{j_1 j'_1} \delta_{j_2 j'_2} (-1)^{j_{1} + j_{2} + j} \tilde{\gamma}_1^{j_1} \tilde{\gamma}_2^{-1} \tag{B23}
\]
Plugging Equation (B23) into (B22) gives us
\[
\langle j_1 j_2; j | \hat{T}_0 \circ \hat{S}_0 | j'_1 j'_2; j' \rangle = \delta_{(j_1,j_2;j')} \delta_{j_1 j'_1} \delta_{j_2 j'_2} (-1)^{j_{1} + j_{2} + j} \frac{\tilde{\gamma}^{j j' j_{2 1}}}{j_1 j_2} \langle j_1 | \hat{T}_0 | j'_1 \rangle \langle j_2 | \hat{S}_0 | j'_2 \rangle \tag{B24}
\]
The Kronecker-delta on \( j_1, j'_1 \) yields zero unless \( j_1 = j'_1 \), and hence we have the simplification
\[
(-1)^{j_{1} + j_{2} + j} \langle j_1 j_2; j | \hat{T}_0 \circ \hat{S}_0 | j'_1 j'_2; j' \rangle = (-1)^{2(j_1 + j_2)} \tag{B25}
\]
Since the \( j_1 \) and \( j_2 \) are half-integers, \( 2(j_1 + j_2) = \text{even} \Rightarrow (-1)^{2(j_1 + j_2)} = +1 \), and by the triangular delta induced by Equation (B23), \( j \in \mathbb{N}_0 \Rightarrow (-1)^{2j} = +1 \). Hence, the phase in Equation (B24) disappears, and restoring the triangle condition completes the proof.

**Corollary B.2.3**

Consider the spherical tensor, \( \hat{T} \), of rank 0. We note that its tensor product with the identity is equivalent to their scalar product, since by Equation (B7) we have
\[
\hat{T}_0 \circ \mathbb{1}_0 = (-1)^0 \mathbb{0} \hat{T}_0 \circ \mathbb{1}_0 \mathbb{0} = \mathbb{0} \hat{T}_0 \circ \mathbb{1}_0 \mathbb{0} = \hat{T}_0 \mathbb{0} \tag{B25}
\]
The last equivalence above comes from Equation (B4) of Example B.1. However, we will use the notation \( \hat{T}_0 \circ \mathbb{1}_0 \) to make it clear that \( \hat{T} \) is an operator acting on the space of particle 1 with \( j'_1 \to j_1 \), WLOG. We can then write the reduced matrix elements of \( \hat{T}_0 \) via
\[
\langle j_1 j_2; j | \hat{T}_0 \circ \mathbb{1}_0 | j'_1 j'_2; j' \rangle = \delta_{(j_1,j_2;j')} \delta_{j_1 j'_1} \delta_{j_2 j'_2} \tilde{\gamma}_1^{j_{2 1}} \langle j_1 | \hat{T}_0 | j'_1 \rangle \tag{B26}
\]
B.4. Decomposition Theorems

By extending Corollary B.2.2, all we have to do to prove Corollary B.2.3 is take $\vec{S}_0 = 1_0$, and substitute Equation (B11) into (B21), et voilà. Corollary B.2.3 will come in handy in the future, but what if we wanted to take the tensor product of the identity with a spherical tensor of an arbitrary rank, for instance?

**Corollary B.2.4**
Consider the spherical tensor product made up of the spherical tensors $\hat{T}_L$ and the identity operator $1_0$. By Equation (B4), this gives back the arbitrary spherical tensor, as expected

$$\hat{T}_{LM} \doteq [1_0 \otimes \hat{T}_L]_{LM}$$

In contrast with the corollaries above, let’s switch to $ls$-coupling, and assume that $j'$ is a half-integer and $l, L \in \mathbb{N}_0$. Then the symmetrized $J$-scheme reduced matrix elements of this tensor product comes to

$$\langle ls:j|||T_L\rangle = -\delta_{ll'} (1)^{l+2s+j+L+s'} \widehat{L}_{j'j} \left\{ \begin{array}{ccc} l & s & j' \\ l' & s' & j' \end{array} \right\} \langle s||\hat{T}_L||s' \rangle$$

(B27)

**Proof of Corollary (B.2.4).**

The first clear step is to input Equation (B4) into Equation (B15) of Theorem B.2, and notationally switch from $jj$-coupling to $ls$-coupling via $\langle j_1 j_2:j \rangle \rightarrow \langle l s:j \rangle$ and $|j_1 j_2:j'\rangle \rightarrow ||l' s':j'\rangle$. With the identity operator of rank 0 and Equation (B12), this gives

$$\langle ls:j|||\hat{T}_L|||l' s':j'\rangle = \delta_{ll'} (1)^{l+2s+j+L+s'} \widehat{L}_{j'j} \left\{ \begin{array}{ccc} l & s & j \\ l' & s' & j' \end{array} \right\} \langle s||\hat{T}_L||s' \rangle$$

(B28)

We notice that the $9j$-symbol above has a zero entry, so now we can use Equation (A38) and then (A39) to reduce the $9j$-symbol down into a $6j$-symbol, as follows (sparing the algebra)

$$\left\{ \begin{array}{ccc} l & s & j \\ l' & s' & j' \\ 0 & L & L \end{array} \right\} = \delta_{ll'} (1)^{l+2s+j+L+s'} \widehat{L}_{j'j} \left\{ \begin{array}{ccc} l & s & j' \\ l' & s' & j' \end{array} \right\} \langle s||\hat{T}_L||s' \rangle$$

(B29)

where we applied Equation (A28), used $(-1)^{2j'} = -1$ since $j'$ is a half-integer, that $(-1)^{3L} = (-1)^{2L} (-1)^L = (-1)^L$ since $L \in \mathbb{N}_0$, and that the $\delta_{ll'}$ sets $\widehat{L}_{j'j} = \widehat{L}_{j'j}^{-1}$ and $(-1)^{2l+l'} = (-1)^{3l} = (-1)^{l}$ since $l \in \mathbb{N}_0$. Plugging Equation (B29) into Equation (B28) will cancel the prefactors of $\widehat{L}$ and $\widehat{L}$, and by taking note of the redundancy of the Kronecker-delta on $l, l'$ and rearranging the phase we retrieve the desired result of Equation (B27).

Theorem B.2 and its subsequent corollaries are useful for decomposing spherical tensor operators when the states involved are already in $J$-scheme. But what about the case when the coupling of the states is not defined a priori? For this case, we must use the following:
B.4. Decomposition Theorems

Theorem B.3
Consider the spherical tensor product made up of the spherical tensors $\hat{A}_{L_1}$ and $\hat{B}_{L_2}$ by

$$\hat{T}_{LM} \equiv \left[ \hat{A}_{L_1} \otimes \hat{B}_{L_2} \right]_{LM}$$

where all of these spherical tensors act on the same Hilbert space spanned by the basis states $\{|\eta J M_J\rangle\}$, and $\eta$ are any additional quantum numbers needed to fully specify the states. We may “insert an identity” into the reduced matrix elements of the tensor product, via completeness, in the form of

$$\langle \eta J \| \hat{T}_L \| \eta' J' \rangle = (-1)^{J + L + J'} \sum_{\eta'', J''} L \left[ \begin{array}{ccc} L_2 & L_1 & L \\ J & J' & J'' \end{array} \right] \langle \eta J \| \hat{A}_{L_1} \| \eta'' J'' \rangle \langle \eta'' J'' \| \hat{B}_{L_2} \| \eta' J' \rangle$$

(B30)

Now you may be thinking, “this is all great, but what if I want the anti-symmetrized versions?” This is important in the case that the quantum mechanical system of interest obeys Fermi-Dirac statistics, which it often will in nuclear physics. The following theorem comes in handy, which can be applied to all the corollaries above:

Theorem B.4
Consider the spherical tensor operator, $\hat{T}_{LM}$, with $J$-scheme reduced matrix elements in $jj$-coupling. We can anti-symmetrize its reduced (or standard) matrix elements using the (analogous) formula, as follows

$$\langle j_1 j_2; j \| \hat{T}_L \| j_1' j_2'; j' \rangle = \langle j_1 j_2; j \| \hat{T}_L \| j_1' j_2'; j' \rangle - (-1)^{j_1 + j_2 - j'} \langle j_1 j_2; j \| \hat{T}_L \| j_2' j_1'; j' \rangle$$

(B31)

noting that the last term of the RHS has a swapping of $j_1' \leftrightarrow j_2'$ compared to the first term, and that the LHS has semicolons as opposed to the RHS which has colons (see the List of Symbols). To normalize Equation (B31), we simply send

$$\langle j_1 j_2; j \| \hat{T}_L \| j_1' j_2'; j' \rangle \longrightarrow \frac{1}{\sqrt{(1 + \delta_{12})(1 + \delta_{1'2'})}} \langle j_1 j_2; j \| \hat{T}_L \| j_1' j_2'; j' \rangle$$

(B32)

The proof of this theorem, and the genesis of the normalization factor in Equation (B32), comes from applying Equation (A22). If you are unsure whether or not your matrix elements are anti-symmetrized, due to notational inconsistencies, the following corollary is a good check:
Corollary B.4.1
Consider the spherical tensor operator, $\hat{T}_{LM}$, as in Theorem B.4. Its anti-symmetrized reduced (or standard) matrix elements obey the following (analogous) formula

$$
\langle j_1 j_2; j |\hat{T}_L||j'_1 j'_2; j'\rangle = -(\frac{-1}{2})^{j'_1 + j'_2 - j'} \langle j_1 j_2; j |\hat{T}_L||j'_1 j'_2; j\rangle
$$

noting the difference in the positions of $j'_1$ and $j'_2$.

Proof of Corollary (B.4.1).

We simply plug Equation (B31) into the RHS of (B33) as so

$$
-(-1)^{j'_1 + j'_2 - j'} \langle j_1 j_2; j |\hat{T}_L||j'_1 j'_2; j'\rangle = -(-1)^{j'_2 + j'_1 - j'} \langle j_1 j_2; j |\hat{T}_L||j'_1 j'_2; j'\rangle + \langle j_1 j_2; j |\hat{T}_L||j'_2 j'_1; j'\rangle
$$

where, in the first equality, we sneakily used the fact that

$$
(-1)^{2(j'_1 + j'_2 - j')} = (-1)^{2(j'_2 + j'_1)} (-1)^{-2j'} = +1 \times (-1)^{2j'} = +1
$$

and in the second line we used Equation (B31) on $\langle j_1 j_2; j |\hat{T}_L||j'_1 j'_2; j'\rangle$, taking careful note of where the $j'_1$ and $j'_2$ are ordered throughout the arithmetic. Notice that this proof would still hold if we had carried the normalization factors throughout the steps, since they would just cancel out from both sides.

*one should also be aware of the appearance of colons or semicolons
Appendix C

Fock Space and Operators

In second quantization, a Fock state is a way of representing a quantum many-body state in terms of a well-defined particle number, as opposed to working with energy eigenstates as in first quantization. That is, we label the many-body state by the occupation number of the single-particle states. In general, we can write

\[ |\Psi_0\{1, \ldots, A\}\rangle = |n_1, \ldots, n_A\rangle \quad (C1) \]

where, for fermions, the state \( \Psi_0 \) is an \( A \)-body Slater determinant (see Section 2.1.3) and \( n_k \) are occupation numbers which are either equal to 0 or 1 for \( \forall k \), due to the Pauli exclusion principle. A simple example is where the single-particle states \( \phi_1 \) and \( \phi_2 \) are both occupied

\[ |1_1, 1_2\rangle = \frac{\phi_1\phi_2 - \phi_2\phi_1}{\sqrt{2}} \]

This shows us the primary advantage of Fock states: we can model quantum many-body physics without any redundant reference to the particle labels.

In Fock space (see Equation (C6) below), we generate the most general state by acting on the vacuum state, \( |0\rangle \), with the fermionic creation operators, \( \hat{c}^\dagger \). So, an equivalent way of writing the Slater determinant \( |\Psi_0\rangle \) in this occupation number representation would be

\[ |n_1, \ldots, n_A\rangle = (\hat{c}_1)^{n_1} \cdots (\hat{c}_A)^{n_A} |0\rangle \]

The annihilation operator is defined by its action on the vacuum giving us nil. That is,

\[ \hat{c}|0\rangle = 0 \iff (\hat{c}|0\rangle)^\dagger = 0^\dagger \iff \langle 0|\hat{c}^\dagger = 0 \quad (C2) \]

We can capture the Dirac-Fermi statistics of fermions with the algebraic structure\(^\dagger\) of the following anti-commutators of creation and annihilation operators

\[ \{\hat{c}_i, \hat{c}_j\} \equiv \hat{c}_i\hat{c}_j + \hat{c}_j\hat{c}_i = 0 \quad (C3) \]
\[ \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} \equiv \hat{c}_i^\dagger\hat{c}_j^\dagger + \hat{c}_j^\dagger\hat{c}_i^\dagger = 0 \quad (C4) \]
\[ \{\hat{c}_i, \hat{c}_j^\dagger\} \equiv \hat{c}_i\hat{c}_j^\dagger + \hat{c}_j^\dagger\hat{c}_i = \delta_{ij} \quad (C5) \]

where we’ve used natural units, so \( \hbar = 1 \). For bosons, we’d have the same algebra, except we’d use commutators instead of anti-commutators. However, in nuclear theory we won’t commonly make reference to bosonic algebra, since protons and neutrons are both fermions.

\(^*\)this represents the state devoid of any particles, i.e., it is empty

\(^\dagger\)referred to as the “algebra” of the QFT by most physicists, which would likely drive a mathematician mad
We call the collection of all possible Fock states the “Fock space.” A more technical way
of describing the fermionic Fock space is that it is the direct sum of all the possible anti-
symmetrized (AS) tensor products of single-particle Hilbert spaces. Symbolically, a Fock space,
$F$, over the Hilbert spaces, $H$, can be represented as

$$F(H) = \bigoplus_n AS(H^{\otimes n}) = C \oplus AS(H) \oplus AS(H \otimes H) \oplus AS(H \otimes H \otimes H) \oplus \ldots \quad (C6)$$

Note that separate Fock spaces can be defined for the protons and neutrons respectively, since
they both constitute different states of the nucleon (see Section 2.2.1). Furthermore, excitations
of these nucleons can be modelled using Fock space in a “particle-hole” occupation number
representation - see Figure 1 of [149], for instance. That is, whereby we can define a Fermi
surface such that our nucleons are packed behind, particle operators $\hat{c}^\dagger_a$ and $\hat{c}_a$
act above the Fermi energy and hole operators $\hat{h}^\dagger_b = \tilde{c}_b$ and $\hat{h}_b = \tilde{c}^\dagger_b$ act below the Fermi energy.*

### C.1 Normal Ordering and Contractions

Let’s consider an arbitrary product of creation and/or annihilation operators, $\hat{a}\hat{b}\hat{c}\hat{d}\hat{e} \ldots$. Because
of Equation (C2), it’s more convenient to deal with this product in a form such that all
the creation operators are put to the left and all the annihilation operators are put to the right.
This is called the “normal ordered” product, which we will denote with our own notation†

$$|\hat{a}\hat{b}\hat{c}\hat{d}\hat{e} \ldots|$$

To evaluate the normal ordered product, we may have to introduce a phase due to the commu-
tation relations in Equations (C3) to (C5). For example, for a three fermion state

$$|\hat{c}_1\hat{c}^\dagger_2\hat{c}^\dagger_3| = -\hat{c}^\dagger_2\hat{c}_1\hat{c}^\dagger_3 = \hat{c}^\dagger_2\hat{c}^\dagger_3\hat{c}_1 = -\hat{c}^\dagger_3\hat{c}^\dagger_2\hat{c}_1$$

Another tool in the context of second quantization is a “(Wick) contraction,” which is
defined as the expectation value of a product with respect to the vacuum (reference) state

$$\bar{a}\bar{b} \equiv \langle 0|\hat{a}\hat{b}|0\rangle \quad (C7)$$

An operator form which will equivalently give Equation (C7) is taken as

$$\bar{a}\bar{b} \doteq \hat{a}\hat{b} - |\hat{a}\hat{b}| \quad (C8)$$

where the normal ordering is defined with respect to the same vacuum, to stay consistent. This
definition seems innocuous at first, but it quickly becomes rather involved. Before exposing
some of these complexities, notice that Equation (C8) corresponds with our intuitive notion of
normal ordering. That is, when taking the expectation value of both sides of the equation

*see Equation (C17) below for the definition of this “tilde” operator

†More common notations within the literature are $N(\cdots)$ or $:\cdots:$, which we find cumbersome and easy
to miss respectively. We chose our new notation because the left bracket and right bracket form an “N” when
elongated and squished together.
C.1. Normal Ordering and Contractions

\[
\langle 0|\hat{a}\hat{b}|0 \rangle = \langle 0|\hat{a}\hat{b}|0 \rangle - \langle 0|\hat{a}\hat{b}|0 \rangle
\]

\[
\langle 0|\hat{a}\hat{b}|0 \rangle \cdot \langle 0|0 \rangle = \langle 0|\hat{a}\hat{b}|0 \rangle - \langle 0|\hat{a}\hat{b}|0 \rangle
\]

(C9)

where the RHS remained unchanged, but we inserted Equation (C7) on the LHS, and then pulled it out since the expectation value is a \( \mathbb{C} \)-number. Generalizing Equation (C9) gives

\[
\langle 0|\hat{a}\hat{b}\hat{c}\hat{d}\hat{e} \cdots |0 \rangle = 0
\]

(C10)

Why is this intuitive? Well, for \( \hat{a}\hat{b}\hat{c}\hat{d}\hat{e} \cdots \), we know that there exists at least one creation or annihilation operator. For the annihilation operator, normal ordering pushes it against the vacuum state, \(|0\rangle\), giving zero by Equation (C2) - and similarly for a creation operator and the bra. Equation (C10) is important, since it can be taken as a defining feature when generalizing the normal ordering to reference states other than the vacuum (see Section 5.3) [12]. Finally, some more involved arithmetic shows that the normal ordering of a contraction is as follows

\[
\hat{a}\hat{b}\hat{c}\hat{d}\hat{e} \cdots \hat{f} \hat{g} \cdots = (-1)^P \hat{b}\hat{e}\hat{d}\hat{g} \hat{a}\hat{c}\hat{f} \hat{h} \cdots
\]

(C11)

where \( P \) counts the number of transpositions required to bring the contracted pairs to the left of the final normal ordered product [5].

C.1.1 Wick’s Theorem

We would like a way to rewrite large strings of creation and annihilation operators in a more manageable form when doing derivations. Wick’s Theorem does just that. It states that an arbitrary product of creation and/or annihilation operators can be rewritten as its normal ordering plus the sum of the normal orderings of all possible pair-wise contractions. Formally:

**Theorem C.1: “Wick’s Theorem”**

Consider the arbitrary product of creation/annihilation operators, \( \hat{a}\hat{b}\hat{c}\hat{d} \cdots \). We can expand this product using normal ordering (as defined above) along with Equation (C11), as follows

\[
\hat{a}\hat{b}\hat{c}\hat{d} \cdots = \hat{a}\hat{b}\hat{c}\hat{d} \cdots
\]

\[
+ \hat{a}\hat{b}\hat{c}\hat{d} \cdots + \hat{a}\hat{b}\hat{c}\hat{d} \cdots + \text{all other 1-contractions}
\]

\[
+ \hat{a}\hat{b}\hat{c}\hat{d} \cdots + \text{all other 2-contractions}
\]

\[
+ \ldots
\]

\[
+ \text{all normal ordered terms of n-contractions}
\]

\[
+ \ldots
\]

\[
+ \text{all normal ordered terms of all possible contractions}
\]

(C12)

This theorem remains valid for any reference state normal ordering, as mentioned in Section 5.3.
C.2 One-Body Operators

In the occupation number representation, we can construct a “one-body operator,” call it $T$, as

$$T = \sum_{\alpha, \beta} t_{\alpha \beta} \hat{c}_\alpha^\dagger \hat{c}_\beta$$

(C13)

where we’ve used the shorthand that a single nucleon $\alpha$ (or $\beta$, etc) has $a \equiv n_a, l_a, s_a, j_a, m_a$.

Why can we do such a thing? For a proof of concept, let’s go ahead and find the operator coefficients $t_{\alpha \beta}$, using Equation (C2) to deduce the fact that

$$\langle \alpha' | \hat{c}_\alpha^\dagger \hat{c}_\beta | \beta' \rangle = \delta_{\alpha \alpha'} \delta_{\beta \beta'}$$

so that sandwiching the operator $T$ with $\langle \alpha' |$ and $| \beta' \rangle$ is

$$\langle \alpha' | T | \beta' \rangle = \sum_{\alpha, \beta} t_{\alpha \beta} \langle \alpha' | \hat{c}_\alpha^\dagger \hat{c}_\beta | \beta' \rangle$$

So overall we can represent a spherical tensor operator, let’s make it rank $L$ with projection-label $M$, by its “one-body matrix elements” (OBMEs) and the creation/annihilation product

$$\hat{T}_{LM} = \sum_{\alpha, \beta} \langle \alpha | \hat{T}_{LM} | \beta \rangle \hat{c}_\alpha^\dagger \hat{c}_\beta$$

(C14)

This can also be proven using Wick’s Theorem, see Example 4.5 of Suhonen [5].

Example C.1

The OBMEs of the number operator are

$$\langle \alpha | \hat{N} | \beta \rangle = \langle \alpha | \eta_\beta | \beta \rangle = \eta_\beta \delta_{\alpha \beta}$$

So, using Equation (C14), the occupation number representation of the number operator is

$$\hat{N} = \sum_{\alpha, \beta} \eta_\beta \delta_{\alpha \beta} \hat{c}_\alpha^\dagger \hat{c}_\beta = \sum_{\alpha} \eta_\alpha \hat{c}_\alpha^\dagger \hat{c}_\alpha = \sum_{\alpha} \hat{c}_\alpha^\dagger \hat{c}_\alpha$$

(C15)

The last step in the line above occurs since, for fermions, the number eigenvalue is $\eta_\alpha = 0$ or $1 \ \forall \alpha$, so we can simply reorder the summation index. In essence, Equation (C15) justifies why we refer to this representation as occupation “number” representation, and it justifies why we’ll commonly think of $\hat{c}_\alpha^\dagger \hat{c}_\alpha$ as a “density” operator.

Using the Wigner-Eckart Theorem in Equation (B9), $\hat{T}$ in (C14) can be rewritten as

$$\hat{T}_{LM} = \sum_{\alpha, \beta} (-1)^{j_a + m_a} \begin{pmatrix} j_a & L \\ -m_a & M \end{pmatrix} \langle j_a | \hat{T}_{LM} | j_b \rangle \hat{c}_\alpha^\dagger \hat{c}_\beta$$

(C16)

* i.e., all the relevant quantum numbers
C.2. One-Body Operators

It so happens that the creation operator is a spherical tensor of rank $j_a$, however the annihilation operator is not! So we’d like to find a form of the annihilation operator that is a spherical tensor, so that we can apply theorems developed in Section B.4 to this operator representation.

**Definition C.1: “Tilde (Annihilation) Operator”**

Consider the standard annihilation operator, $\hat{c}_a \equiv \hat{c}_{j_a,m_a}$, which kills the particle (field excitation) $a$. Then, for future convenience, we make the definition

$$\tilde{c}_a \equiv (-1)^{j_a+m_a} \hat{c}_{-a} \text{ where } \hat{c}_{-a} \equiv \hat{c}_{j_a,-m_a}$$

(C17)

**Remark C.1**

The tilde operator, $\tilde{c}_a$, and the creation operator, $\hat{c}^\dagger_a$, are both spherical tensors of rank $j_a$, whereas the annihilation operator is not spherical tensor operator. For proof of this statement, see the work leading up to Equation (A.81) and (A.82) of [171].

Now we have a mechanism to turn the density in Equation (C16) into a spherical tensor, which we’ll do via a tensor product, as defined by Equation (B3). We may do this with confidence considering Remark C.1, and so

$$[\hat{c}^\dagger_a \otimes \tilde{c}_b]_{LM} = \sum_{m_a m_b} (j_a m_a j_b m_b \mid L M) \hat{c}^\dagger_a \tilde{c}_b$$

(C18)

Let’s see if we can massage Equation (C18) out of (C16). By Equation (A26) and (A23), we can rearrange the $3j$-symbol from (C16) as

$$\begin{pmatrix} j_a & L & j_b \\ -m_a & M & m_b \end{pmatrix} = (-1)^{-2j_b-L-M} \hat{L}^{-1}(j_a, -m_a j_b m_b \mid L, -M)$$

(C19)

Equation (C19) turns (C16) into

$$\hat{T}_{LM} = \sum_{j_a j_b m_a m_b} (-1)^{j_a-m_a-2j_b-L-M} \hat{L}^{-1}(j_a, -m_a j_b m_b \mid L, -M) \langle j_a \mid [\hat{T}_L] \mid j_b \rangle \hat{c}^\dagger_a \tilde{c}_b$$

(C20)

Notice that since $m_b$ runs over $-j_b, -j_b+1, \ldots, j_b-1, j_b$, we can simply run $m_b$ backwards within the sum, and get the equivalent result in Equation (C20). Hence

$$\hat{T}_{LM} = \sum_{j_a j_b m_a m_b} (-1)^{j_a-m_a-2j_b-L-M} \hat{L}^{-1}(j_a, -m_a j_b m_b \mid L, -M) \langle j_a \mid [\hat{T}_L] \mid j_b \rangle \hat{c}^\dagger_a \tilde{c}_b$$

where we used Equation (A10) in the second line above. To recover the tilde operator, we use Definition (C.1) with $\tilde{c}_b \equiv (-1)^{-j_b-m_b} \tilde{c}_b$, which give us
C.3 Two-Body Operators

\[ \hat{T}_{LM} = \sum_{j_a j_b m_a m_b} (-1)^{j_a + m_a + j_b + m_b - 2L - M} \hat{L}^{-1} \langle j_a | \hat{T}_L | j_b \rangle \langle j_a m_a j_b m_b | L M \rangle e_{a}^{\dagger} e_{b} \quad (C21) \]

In the sum over \( m_a, m_b \), the CG coefficients will yield a zero unless they satisfy Condition (A3), hence we must have that \( m_a + m_b = M \), and so

\[ \Rightarrow (-1)^{-m_a - m_b - M} \equiv (-1)^{2(-m_a - m_b)} = (+1)^{-(m_a + m_b)} = +1 \quad (C22) \]

Likewise, we notice that

\[ (-1)^{2j_a - 2j_b - 2L} = (-1)^{2(j_a - j_b)} (+1)^{-L} = +1 \quad (C23) \]

Remarkably, by using Equation (C22) and (C23), the phase in Equation (C21) disappears

\[ \hat{T}_{LM} = \hat{L}^{-1} \sum_{j_a j_b} \langle j_a | \hat{T}_L | j_b \rangle \sum_{m_a m_b} \langle j_a m_a j_b m_b | L M \rangle e_{a}^{\dagger} e_{b} \quad (C24) \]

And now, comparing Equation (C24) with (C18), you can see that everything has been perfectly cooked, and we may write the compact version as

\[ \hat{T}_{LM} = \hat{L}^{-1} \sum_{a, b} \langle a | \hat{T}_L | b \rangle [e_{a}^{\dagger} \otimes e_{b}]_{LM} \quad (C25) \]

Finally, consider sandwiching \( \hat{T}_{LM} \) with some general final state \( \langle \eta_f J_f M_f | \) and initial state \( | \eta_i J_i M_i \rangle \), where the labels \( \eta_f, \eta_i \) represent any additional quantum numbers we would need to fully characterize the quantum mechanical system of interest. Reducing both sides gives

\[ \langle f | \hat{T}_L | i \rangle = \hat{L}^{-1} \sum_{a, b} \langle a | \hat{T}_L | b \rangle \langle \eta_f J_f | [e_{a}^{\dagger} \otimes e_{b}]_{LM} | \eta_i J_i \rangle \quad (C26) \]

where we’ve introduced the notation \( \langle f \rangle \equiv \langle \eta_f J_f | \) and \( | i \rangle \equiv | \eta_i J_i \rangle \), for simplicity. We call Equation (C26) the “transition amplitude,” and the \( \langle \eta_f J_f | [e_{a}^{\dagger} \otimes e_{b}]_{LM} | \eta_i J_i \rangle \) pieces are referred to as the “one-body transition densities” (OBTDs). In the context of nuclear physics, a transition amplitude is commonly called a “nuclear matrix element” (NME). For example, Equation (C26) could describe the decay of a nucleus from its initial state to a final state in terms of looping over its constituent nucleons (as labelled by \( a, b \)).

C.3 Two-Body Operators

We will now construct the analogous formula of Equation (C26) for the case of a “two-body operator.” A two-body operator acts on two particles; let’s associate the sets of quantum numbers for two particles in the ket as \( c \) and \( d \), and then \( a \) and \( b \) for the corresponding bra. For example, in a hypothetical nuclear reaction, we might be turning particle 1 from the neutron state \( c \) into the proton state \( a \), and then particle 2 may undergo an electromagnetic transition from \( d \) to \( b \). We can express this two-body operator as a spherical tensor, \( \hat{T}_{LM} \), by
\[ \hat{T}_{LM} = \sum_{abcd} \langle a, b | \hat{T}_{LM} | c, d \rangle \, \hat{c}_a^\dagger \hat{c}_{b}^\dagger \hat{c}_c \hat{c}_d \]  \tag{C27}

where the two-body matrix elements (TBMEs) of \( \hat{T} \) are naturally in \( M \)-scheme. Note that the order of the creation/annihilation product has been determined in the same manner which was used to obtain Equation (C14), and that the index \( c \) is distinct from the label \( \hat{c} \) for \( \hat{c}_c \).

First by switching \( M \)-scheme to \( J \)-scheme in the TBMEs, then using similar algebra to Section C.2 above, whilst strategically applying Equations (A2), (B3), and (C17), one can show that Equation (C27) may be rewritten as

\[ \hat{T}_{LM} = \hat{L}^{-1} \sum_{abcd} \sum_{J_{ab}, J_{cd}} \langle a b : J_{ab} | \hat{T}_L | c d : J_{cd} \rangle \left[ [\hat{c}_a^\dagger \otimes \hat{c}_{b}^\dagger]_{J_{ab}} \otimes [\hat{c}_c \otimes \hat{c}_d]_{J_{cd}} \right]_{LM} \]  \tag{C28}

As with Equation (C25), we can construct the NME of (C28) by sandwiching it between a final and initial nuclear state and then reducing both sides, giving

\[ \langle f | \hat{T}_L | i \rangle = \hat{L}^{-1} \sum_{abcd} \sum_{J_{ab}, J_{cd}} \langle a b : J_{ab} | \hat{T}_L | c d : J_{cd} \rangle \times \langle \eta_J | f \rangle \left[ [\hat{c}_a^\dagger \otimes \hat{c}_{b}^\dagger]_{J_{ab}} \otimes [\hat{c}_c \otimes \hat{c}_d]_{J_{cd}} \right]_L \langle \eta_J | i \rangle \]  \tag{C29}

The piece after the TBMEs within the sum are called the “two-body transition densities” (TBTDs). To calculate the TBTDs, we will use a code called nutbar (see Section 6.3). Intuitively, we’d like to be able to relate the TBTDs to the OBTDs of Equation (C26). We can accomplish this by applying Equation (B30) of Theorem B.3 to Equation (C29), to obtain

\[ \langle f | \hat{T}_L | i \rangle = (-1)^{J_f + L + J_i} \sum_{abcd} \sum_{J_{ab}, J_{cd}} \left\{ \begin{array}{ccc} J_{cd} & J_{ab} & L \\ J_f & J_i & J_k \end{array} \right\} \langle a b : J_{ab} | \hat{T}_L(k) | c d : J_{cd} \rangle \times \langle \eta_J | f \rangle \left[ [\hat{c}_a^\dagger \otimes \hat{c}_{b}^\dagger]_{J_{ab}} \otimes [\hat{c}_c \otimes \hat{c}_d]_{J_{cd}} \right]_L \langle \eta_J | i \rangle \]  \tag{C30}

There are several important points to make about Equation (C30) before we move on. First, notice that inserting an identity has physically introduced an “intermediate” nuclear state, denoted by \( k \). For instance, if we consider double-beta decay of Calcium-48 (for more on this see Chapter 3), the initial, intermediate, and final nuclear states are

\[ |i\rangle = |^{48}\text{Ca}\rangle, \quad |k\rangle = |^{48}\text{Sc}\rangle, \quad \text{and,} \quad |f\rangle = |^{48}\text{Ti}\rangle \]

Another contrast between Equation (C29) and (C30) is that the latter has incorporated the fact that the spherical tensor operator, \( \hat{T} \), could depend on the structure of the intermediate state. Hence, we made the relabelling \( \hat{T}_L \rightarrow \hat{T}_L(k) \) within the TBMEs, which will be discussed more in Section C.3.1 below. Finally, we see that the OBTDs of Equation (C30) do not exactly match the form of the OBTDs of Equation (C26). To get an exact match of the OBTDs, one could imagine using Equation (B6) on (C29) before inserting an identity via Equation (B30).

---

* this can be proven using Equation (C12) of Wick’s Theorem

† The sum with respect to \( k \) has been appended to the leftmost summation symbol of Equation (C30), which we point out in contrast to Equation (C29).
C.3. Two-Body Operators

Example C.2
Let’s now push Example B.2 from its OBME version to its TBME version. Such TBMEs would be useful in an Equation like (C30) above. First, we recall from Equation (A20) that
\[
\langle j_1 j_2; j m | j_3 j_4; j' m' \rangle = \delta_{jj'} \delta_{mm'} \left[ \delta_{13} \delta_{24} - (-1)^{j_3+j_4-j'-j} \delta_{14} \delta_{23} \right]
\]

It’s easy to argue that the only thing to do in order to switch from \( \langle j_1 j_2; j m | j_3 j_4; j' m' \rangle \rightarrow \langle j_1 j_2; j | i | j_3 j_4; j' \rangle \) is to include a factor of \( \hat{U} \). This hat factor is induced in the same manner as it was for Equation (B11), with the small caveat that we must properly couple \( \eta = j_1 j_2 \) to \( j \) and \( \eta' = j_3 j_4 \) to \( j' \) in the Wigner-Eckart Theorem. Finally, since we are using the reduced matrix elements, there is no need to include the \( \delta_{mm'} \) from Equation (A20). We obtain
\[
\langle j_1 j_2; j | i | j_3 j_4; j' \rangle = \delta_{jj'} \left[ \delta_{13} \delta_{24} - (-1)^{j_3+j_4-j'-j} \delta_{14} \delta_{23} \right] \hat{U}
\] (C31)

Note that we could prove this formally by using Equation (B15) with \( 1_{00} \rightarrow [1_0 \otimes 1_0]_{00} \) and the appropriate identities, and then anti-symmetrizing via Theorem B.4.

C.3.1 The Closure Approximation
Mathematically, we arrived at Equation (C30) by applying Theorem B.3 to Equation (C29), but this introduced the intermediate state \( k \). At this point, we were forced to admit that the two-body operator itself could depend on the intermediate state, and hence we wrote \( \hat{T}_L(k) \) in the TBMEs. So, physically, in order to recover Equation (C29) when starting with the more general result of (C30), we have to guarantee that the two-body operator is independent of \( k \) - so that the sum over \( k \) can be performed by reversing Equation (B30) of Theorem B.3.

Some operators are naturally independent of \( k \), but many are not.* In the unfortunate case that an operator has a complicated dependence on \( k \), theorists will often impose an approximation that enforces an independence
\[
\hat{T}_L(k) \rightarrow \hat{T}_L
\] (C32)

We will refer to the utilization of Equation (C32) as making a “closure approximation.” This nomenclature comes from its use in neutrinoless double-beta decay, where the operators involved will be “closed off” from their dependence on the intermediate nuclear state of the decay. Under such an approximation, or an exact guarantee of a spherical tensor’s independence of the intermediate state, we may sum over \( k \) and transform Equation (C30) into Equation (C29), which we copy here for the reader’s convenience
\[
\langle f|\hat{T}_L|i \rangle = \hat{L}^{-1} \sum_{abcd} \sum_{J_{ab} J_{cd}} \langle a b; J_{ab} || \hat{T}_L || c d; J_{cd} \rangle \times \langle \eta_f J_f || \left[ \hat{c}_a^\dagger \otimes \hat{c}_b^\dagger \right]_{J_{ab}} \otimes \left[ \hat{c}_c \otimes \hat{c}_d \right]_{J_{cd}} || \eta_i J_i \rangle
\] (C33)

*see, for instance, the operator structure of neutrinoless double-beta decay in Section 4.1
Appendix D

Summation Limits for the Talmi-Moshinsky Transformation

To get the summation limits for Equation (2.9), let’s consider the bracket

\[ D_{12} \equiv \langle n_r, \Lambda; L|l_1, n_2; L \rangle \]

By Equation (2.7), we have \( \Delta(l_r \Lambda; L) \) and \( \Delta(l_2; L) \), hence

\[ |l_r - \Lambda| \leq L \leq l_r + \Lambda \quad \text{and} \quad |l_1 - l_2| \leq L \leq l_1 + l_2 \]  \hspace{1cm} (D1)

Now, the trick is to consider the energies from Equation (2.2), \( E_{nl}[\hbar \omega] = 2n + l + 3/2 \), which apply since the Talmi-Moshinsky brackets are constructed in the oscillator basis. Let’s define something akin to the total energies of the lab frame and the relative/CoM coordinates

\[ \epsilon_{12} \equiv 2n_1 + l_1 + 2n_2 + l_2 \]  \hspace{1cm} (D2)

and,

\[ \epsilon_{rc} \equiv 2n_r + l_r + 2N + \Lambda \]  \hspace{1cm} (D3)

Why did we drop the 3/2’s? Well, by invoking conservation of energy we’d have \( E_{12} = E_{rc} \), or using the definitions in Equation (D2) and Equation (D3), equivalently

\[ \epsilon_{12} = \epsilon_{rc} \implies 2n_1 + l_1 + 2n_2 + l_2 = 2n_r + l_r + 2N + \Lambda \]  \hspace{1cm} (D4)

Physically, it’s clear that the inherent energy content contained in particles 1 and 2 has to be the same in the lab frame as it is in the relative/CoM coordinates. This implies that, given the restriction in Equation (D4) does not hold, then the bracket vanishes

\[ \epsilon_{12} \neq \epsilon_{rc} \implies D_{12} = 0 \]  \hspace{1cm} (D5)

Since \( \epsilon_{12} \) will be set independent from the Talmi-Moshinsky transformation, as far as we’re concerned it is just a constant. Hence, Equation (D5) is actually a constraint which will reduce the size of the summation from Equation (2.9). WLOG, let’s choose to isolate the indices in the order: \( \Lambda, l_r, N, n_r \). Isolating \( \Lambda \) from Equation (D4) gives the constraint

\[ \Lambda = \epsilon_{12} - 2(n_r + N) - l_r \]  \hspace{1cm} (D6)

and we may now write
Appendix D. Summation Limits for the Talmi-Moshinsky Transformation

\[
\sum_{n_s l_r} = \sum_{l_r} \sum_{N, n_r} \Lambda = \epsilon_{12} - 2(n_r + N) - l_r
\]  

(D7)

since the brackets within the sum will obey Equation (D5).

We started with four unknowns, and used one equation to reduced down to three unknowns; so we need to produce three more equations. Notice that the left triangle condition in Equation (D1) actually gives us two equations

\[
L \leq l_r + \Lambda
\]

and,

\[
|l_r - \Lambda| \leq L \implies -L \leq l_r - \Lambda \leq L
\]

(D8)

By adding \(\Lambda + l_r\) to both sides of Equation (D9) and then inserting (D6) we get

\[
\epsilon_{12} - 2(n_r + N) - L \leq 2l_r \leq L + \epsilon_{12} - 2(n_r + N)
\]

\[
\implies \left[ \frac{\epsilon_{12} - L}{2} \right] - (n_r + N) \leq l_r \leq \left[ \frac{\epsilon_{12} + L}{2} \right] - (n_r + N)
\]

(D10)

Note that even though \(\epsilon_{12}, L \in \mathbb{N}_0\), \(\epsilon_{12} \pm L\) need not be divisible by 2. Hence, to get the nearest integer limits, we grabbed the maximal lower bound and the minimal upper bound; so we use the ceiling and floor functions respectively in Equation (D10), for clarity within the summation.

All that’s left to determine is the sum over \(n_r\) and \(N\), which we can get from putting Equation (D6) into (D8) and manipulating

\[
L \leq l_r + \left[ \epsilon_{12} - 2(n_r + N) - l_r \right] = \epsilon_{12} - 2(n_r + N)
\]

\[
L - \epsilon_{12} \leq -2(n_r + N) \implies n_r + N \leq \left[ \frac{\epsilon_{12} - L}{2} \right]
\]

(D11)

noting that \(\epsilon_{12} \geq L\) by Equation (D4). We want to separate out \(n\) and \(N\) into their own sums, which can be done by noticing that, for \(a, b, c \in \mathbb{N}_0\) and some arbitrary \(f(a, b)\), we can write

\[
\sum_{a+b \leq c} f(a, b) = f(0, 0) + f(0, 1) + ... + f(0, c)
\]

\[
+ f(1, 0) + f(1, 1) + ... + f(1, c - 1)
\]

\[
+ ... + f(c - i, 0) + f(c - i, 1) + ... + f(c - i, i)
\]

\[
+ ... + f(c - 1, 0) + f(c - 1, 1)
\]

\[
+ f(c, 0)
\]

\[
= \sum_{b=0}^{c} f(0, b) + \sum_{b=0}^{c-1} f(1, b) + ... + \sum_{b=0}^{i} f(c - i, b) + ... + \sum_{b=0}^{1} f(c - 1, b) + \sum_{b=0}^{0} f(c, b)
\]

\[
= \sum_{b=0}^{c-a} \sum_{a=0}^{c} f(a, b)
\]

123
Or, by switching notation, this shows that Equation (D11) gives us
\[
\sum_{n_r,N=0}^{n_r+N=\lfloor (\epsilon_{12}-L)/2 \rfloor} \sum_{l'_r=\lfloor (\epsilon_{12}-L)/2 \rfloor-n_r}^{\lfloor (\epsilon_{12}-L)/2 \rfloor} \sum_{l_l} \equiv \sum_{N=0}^{\lfloor (\epsilon_{12}-L)/2 \rfloor} \sum_{n_r=0}^{\lfloor (\epsilon_{12}-L)/2 \rfloor} \sum_{n_r,N=0}
\]
\[\text{(D12)}\]

Finally, putting Equation (D10) and (D12) into Equation (D7) yields
\[
\sum_{n_l,l_r,n_r,N=0}^{n_l+l_r,N} \equiv 
\begin{cases} 
\sum_{(4)l_r=\lfloor (\epsilon_{12}-L)/2 \rfloor-n_r} \sum_{(3)N=0}^{\lfloor (\epsilon_{12}-L)/2 \rfloor} \sum_{(2)n_r=0}^{\lfloor (\epsilon_{12}-L)/2 \rfloor} \\
\text{with the constraints: } (5) \Delta = \epsilon_{12} - 2(n_r+N) - l_r, \\ (1) \Delta(l_l,l_r;L) \\
\epsilon_{12} \equiv 2n_1 + l_1 + 2n_2 + l_2 
\end{cases}
\]
\[\text{(D13)}\]

where we’ve appended the definition of \(\epsilon_{12}\) from Equation (D2), and included the coupling on the RHS of (D2), for clarity. For further explicitness, the left superscripts, \((i)\) for \(i = 1, 2, \ldots\), denote the order that each parameter in the limits is set, depending on one another. We will often refer to Equation (D13) and alike as our “chosen Talmi-Moshinsky limits” (CTML), since there are many different ways of writing them. A nice proof of concept is to check that Equation (D13) indeed reproduces Table 1 of [172].

Another necessary exercise is to extend our CTML to the summation limits in Equation (2.11); we’ll start by analyzing (2.20). The derivation of Equation (D13) was performed using conservation of energy between \(\epsilon_{12}\) and \(\epsilon_{rc}\), so with the additional coordinates \(n'_l, l'_r\) (as defined between particles with \(n'_l, l'_l\) and \(l'_2, l'_2\) respectively), we must introduce new information
\[
\epsilon'_{12} \equiv 2n'_l + l'_l + 2n'_r + l'_r + 2N + \Lambda 
\]
\[\text{(D14)}\]

For Equation (2.20), we may take advantage of the \(\delta_{l_l,l_r}\) employed in its proof, giving
\[
\epsilon'_{12} = 2n'_l + l_r + 2N + \Lambda \text{ via, } \delta_{l_l,l_r} 
\]
\[\text{(D15)}\]

Quantization gives us the physical limitation that \(n'_l \in \mathbb{N}_0\), and additionally \(l_r, N, \Lambda\) have all been set for Equation (D13) using the conservation of energy in Equation (D4). So, isolating for \(n'_l\) from Equation (D15) by subtracting it from (D4) gives the constraint
\[
\epsilon'_{12} - \epsilon_{12} = 2(n'_r - n_r) \implies n'_r = \frac{\epsilon'_{12} - \epsilon_{12}}{2} + n_r \in \mathbb{N}_0 
\]

Since we have introduced particles 1’ and 2’, we must also ensure that their angular momenta are appropriately coupled to the total angular momentum, \(L\), via \(\Delta(l'_1, l'_2; L)\). Thus, for the CTML of Equation (2.20), we combine the above constraints with Equation (D13) to obtain
\[
\sum_{n_l,l_r,n'_r,N=0}^{n_l+l_r,N} \equiv 
\begin{cases} 
\sum_{(6)l_r=\lfloor (\epsilon_{12}-L)/2 \rfloor-n_r} \sum_{(5)N=0}^{\lfloor (\epsilon_{12}-L)/2 \rfloor} \sum_{(3)n_r=0}^{\lfloor (\epsilon_{12}-L)/2 \rfloor} \\
\text{with the constraints: } (2) \Delta(l'_l,l'_r;L), \\ (1) \Delta(l_l,l_r;L), \\ (7) \Lambda = \epsilon_{12} - 2(n_r+N) - l_r, \\ (4) n'_r = (\epsilon'_{12} - \epsilon_{12})/2 + n_r \in \mathbb{N}_0 \\
\epsilon_{12} \equiv 2n_1 + l_1 + 2n_2 + l_2, \quad \epsilon'_{12} \equiv 2n'_l + l'_l + 2n'_r + l'_r 
\end{cases}
\]
\[\text{(D16)}\]
Appendix D. Summation Limits for the Talmi-Moshinsky Transformation

Finally, to extend Equation (D16) further to encompass the limits in (2.11), we now must account for: \( l'_r \neq l_r \) and \( L \rightarrow \Delta(l_1 l_2 : L), \Delta(l'_1 l'_2 : L') \). Taking the difference of the conservation of energy in Equation (D14) and (D4) yields

\[
\epsilon'_{12} - \epsilon_{12} = 2(n'_r - n_r) + l'_r - l_r
\]

\[(D17)\]

Since \( n_r \) and \( l_r \) have both been set, all we need to do is set \( l'_r \) and then we may isolate for \( n'_r \) as a constraint. Now that we’ve introduced \( L' \), which is coupled to \( l' \) and \( 2' \), we must also guarantee that it is coupled to the relative/CoM coordinates, via \( \Delta(l'_r \Lambda : L') \). It is straightforward to convince oneself, in this case, that

\[
|l'_r - \Lambda| \leq L' \leq l'_r + \Lambda \implies |\Lambda - L'| \leq l'_r \leq \Lambda + L'
\]

\[(D18)\]

Now that the summation limits over \( l'_r \) have been set, and since \( \Lambda \) is known from Equation (D6), we isolate the constraint for \( n'_r \) from (D17) to obtain

\[
n'_r = \frac{\epsilon'_{12} - \epsilon_{12}}{2} + \frac{l_r - l'_r}{2} + n_r \in \mathbb{N}_0
\]

\[(D19)\]

Equation (2.11) is unique in that we can also skip parts of the summation where the 6\(j\)-symbol vanishes. Hence, via Equation (A27), we obtain

\[
\begin{pmatrix} l \quad l_r \quad \Lambda \\ l'_r \quad L' \quad R \end{pmatrix} = 0 \text{ unless, } \begin{cases} \Delta(l_r L : \Lambda), \Delta(l'_r L' : \Lambda) \\ \Delta(l_r L'_r : R), \Delta(L L'_r : R) \end{cases}
\]

\[(D20)\]

where \( R \) is the rank of the spherical tensor operator. The top two triangle conditions of Equation (D20) have already been implemented above, so only the bottom two need to be added as constraints. Overall, putting Equations (D18), (D19), (D20), and (D16) together gives the CTML for Equation (2.11) as follows

\[
\sum_{n_r l_r, n'_r l'_r, NA} = \sum_{(8) l'_r = |\Lambda - L'| (6) l_r = [(\epsilon_{12} - L)/2] - (n_r + N)} \sum_{(5) N = 0} \sum_{(4) n_r = 0} \begin{cases} \Lambda + L' \text{ \quad } [(\epsilon_{12} + L)/2] - (n_r + N) \\ \text{with the constraints: } (9) \Delta(l_r l'_r : R), (3) \Delta(L L'_r : R), (2) \Delta(l'_r L'_r : L'), (1) \Delta(l r l'_r : L), \\ (10) n'_r = (\epsilon'_{12} - \epsilon_{12})/2 + (l_r - l'_r)/2 + n_r \in \mathbb{N}_0, (7) \Lambda = \epsilon_{12} - 2(n_r + N) - l_r, \\ \epsilon_{12} = 2n_1 + l_1 + 2n_2 + l_2, \epsilon'_{12} = 2n'_1 + l'_1 + 2n'_2 + l'_2 \end{cases}
\]

\[(D21)\]

We remind the reader that the primed quantum numbers are associated with the ket, the unprimed quantum numbers are associated with the bra, and the bolded, parenthesized, left superscripts denote the order that each parameter in the limits should be set. An alternative constraint on \( n'_r \) which yields equivalent results is: \( n'_r = (\epsilon'_{12} - l'_r - \Lambda)/2 - N \in \mathbb{N}_0 \).
Appendix E

Derivation of Equation (D11) from PRC.88.064312(2013)

With 20/20-hindsight, we will want to deal with the integrals
\[ \int_{0}^{\infty} dr r^d e^{-\nu r^2} j_\rho(qr) \] (E1)
where \( d, \rho \in \mathbb{N}_0, \nu \in \mathbb{R}, \) and \( j \) is a spherical Bessel’s function as in Equation (F5). It is well known that
\[ j_n(x) \equiv \ldots = \frac{\pi}{2x} J_{n + \frac{1}{2}}(x) \] (E2)
where \( J \) is a Bessel’s function as in Equation (F4). Hence, using Equation (E2), we may rewrite Equation (E1) as
\[ \int_{0}^{\infty} dr r^d e^{-\nu r^2} j_\rho(qr) = \frac{\pi}{2q} \int_{0}^{\infty} dr r^{d - \frac{1}{2}} e^{-\nu r^2} J_{\rho + \frac{1}{2}}(qr) \] (E3)

As was done in [118], we can solve this from a standard integral table. For instance, in [173] from Equation (6.631) on page 716, it’s stated that
\[ \int_{0}^{\infty} dx \, x^\mu e^{-\alpha x^2} J_\nu(\beta x) = \frac{\Gamma\left(\frac{\mu+\nu+1}{2}\right)}{\beta^2 \alpha^\frac{\mu}{2} \Gamma(\nu + 1)} e^{-\frac{\beta^2}{4\alpha}} M_{\mu, \nu}(z) \] (E4)
where, \( z \equiv \frac{\beta^2}{4\alpha} \) and, \( \text{Re}(\alpha) > 0, \text{Re}(\mu + \nu) > -1 \)
where \( M \) is a Whittaker function as in Equation (F6). Using Equations (8.972.1) and (9.220.2), on pages 1027 and 1059 of [173] respectively, it can easily be shown that
\[ M_{a,b}(x) \equiv x^{b+\frac{1}{2}} e^{-\frac{x}{2}} \left(\frac{a+b-\frac{1}{2}}{a-b-\frac{1}{2}}\right)^{-1} L^{2b}_{a-b-\frac{1}{2}}(x) \] (E5)
where \( L \) are Laguerre polynomials as in Equation (F3), and the coefficient out front is the reciprocal of the generalized binomial coefficient as defined in Equation (F2). Hence, using Equation (E5) and switching \( a \rightarrow \frac{\mu}{2}, b \rightarrow \frac{\nu}{2} \), we can write that
\[ M_{\frac{\mu}{2}, \frac{\nu}{2}}(z) \equiv z^{\frac{\mu+1}{2}} e^{-\frac{\mu}{2}} \left(\frac{\mu+\nu-1}{\mu-\nu-1}\right)^{-1} L^{\nu}_{\mu-\nu-1}(z) \] (E6)
Plugging Equation (E6) into Equation (E4), we see that
Appendix E. Derivation of Equation (D11) from PRC.88.064312(2013)

\[ \int_0^\infty dx x^\mu e^{-\alpha x^2} J_\nu(\beta x) = \frac{\Gamma\left(\frac{\mu+\nu+1}{2}\right)}{\beta \alpha^{\frac{\mu}{2}} \Gamma(\nu+1)} z^{\frac{\nu+1}{2}} \left(\frac{\mu-\nu-1}{2}\right)^{-1} e^{-z L_{\mu+\nu-1}^\nu(z)} \] (E7)

Now, let’s rewrite Equation (E7) in the notation relevant to Equation (E3), by switching

\[ x \to r, \mu \to d - \frac{1}{2}, \alpha \to \nu, \nu \to \rho + \frac{1}{2}, \beta \to q \]

which gives

\[ \int_0^\infty dr r^{d-\frac{1}{2}} e^{-\nu r^2} J_{\rho + \frac{1}{2}}(qr) = \frac{\Gamma\left(\frac{d+\rho+1}{2}\right)}{q \nu^{\frac{d}{2}-\frac{1}{4}} \Gamma(\rho + \frac{3}{2})} z^{\frac{\rho + 1}{2}} \left(\frac{d-\rho-2}{4}\right)^{-1} e^{-z L_{d-\rho-2}^{\rho+\frac{1}{2}}(z)} \] (E8)

where, \( z = \frac{q^2}{4\nu} \) and, \( \text{Re}(\nu) > 0, \text{Re}(d + \rho) > -1 \)

Here let’s introduce the convenient constant

\[ \kappa = d - \rho - \frac{2}{2} \]

so that we can rewrite Equation (E8) as

\[ \int_0^\infty dr r^{d-\frac{1}{2}} e^{-\nu r^2} J_{\rho + \frac{1}{2}}(qr) = \frac{z^{\frac{\rho + 1}{2}} \Gamma\left(\rho + \frac{3}{2}\right)}{q \nu^{\frac{d}{2}-\frac{1}{4}} \Gamma(\rho + \frac{3}{2})} \left(\kappa + \rho + \frac{1}{2}\right)^{-1} e^{-z L_{d-\rho-2}^{\rho+\frac{1}{2}}(z)} \] (E9)

Things are looking really messy, but there is hope! Recall that, for \( t \in \mathbb{R} \) and any \( n \in \mathbb{R} \) such that \( t + n > 0 \), the Gamma function obeys the recurrence formula

\[ \frac{\Gamma(t + n)}{\Gamma(t)} = t(t + 1) \cdots (t + n - 1) \] (E10)

Also, with even more 20/20-hindsight, using Equation (F2), we find that

\[ \binom{t + n - 1}{n} = \frac{(t + n - 1)(t + n - 2) \cdots (t + n - 1) - n + 1}{n!} = \frac{(t + n - 1)(t + n - 2) \cdots t}{n!} = \frac{t(t + 1) \cdots (t + n - 1)}{n!} \] (E11)

So putting together Equation (E10) and (E11) gives

\[ \frac{\Gamma(t + n)}{\Gamma(t)} \cdot \left(\frac{t + n - 1}{n}\right)^{-1} = n! \] (E12)

At this point we can see the trick; let’s take \( t = \rho + \frac{3}{2} \) and \( n = \kappa \) in Equation (E12), so that

\[ \frac{\Gamma\left(\rho + \frac{3}{2} + \kappa\right)}{\Gamma\left(\rho + \frac{3}{2}\right)} \left(\rho + \frac{3}{2} + \kappa - 1\right)^{-1} = \frac{\Gamma\left(\rho + \frac{3}{2} + \kappa\right)}{\Gamma\left(\rho + \frac{3}{2}\right)} \left(\kappa + \rho + \frac{1}{2}\right)^{-1} = \kappa! \] (E13)

Additionally, since \( z = \frac{q^2}{4\nu} \), it’s clear that

127
Appendix E. Derivation of Equation (D11) from PRC.88.064312(2013)

\[ \frac{z^{\frac{3}{4}}}{q \sqrt{\nu}} = \frac{q^{\frac{3}{4}}}{4^{\frac{3}{4}} \nu \frac{d}{2} \cdot q \nu^{\frac{d}{2} - \frac{1}{4}}} = \frac{q^{\frac{1}{2}}}{2^{\frac{3}{2}} \nu^{\frac{d}{2} - \frac{1}{4}}} = \nu^{-\frac{d-1}{2}} \sqrt{q} \]  

(E14)

Now we can simplify Equation (E9) greatly, by plugging in Equation (E13) and E14 to obtain

\[ \int_0^\infty dr \, r^{d-\frac{1}{2}} e^{-\nu r^2} J_{\rho + \frac{1}{2}}(qr) = \nu^{-\frac{d-1}{2}} \sqrt{\frac{q}{8}} \kappa! z^\frac{d}{2} e^{-z} L_{\kappa + \frac{1}{2}}(z) \]  

(E15)

Finally, after much manipulation, we can evaluate the integral of interest, by putting Equation (E15) into Equation (E3), giving

\[ \int_0^\infty dr \, r^{d} e^{-\nu r^2} j_\rho(qr) = \sqrt{\frac{\pi}{2q}} \times \nu^{-\frac{d-1}{2}} \sqrt{\frac{q}{8}} \kappa! z^\frac{d}{2} e^{-z} L_{\kappa + \frac{1}{2}}(z) \]

Or, overall

\[ \int_0^\infty dr \, r^{d} e^{-\nu r^2} j_\rho(qr) = \nu^{-\frac{d-1}{2}} \sqrt{\frac{\pi}{4}} \kappa! z^\frac{d}{2} e^{-z} L_{\kappa + \frac{1}{2}}(z) \]  

(E16)

where, \( z = \frac{q^2}{4\nu} \) and, \( \kappa = \frac{d - \rho - 2}{2} \)

This formula indeed corresponds to Equation (D11) of [118], with the notational identifications that: \( m \leftrightarrow d \), \( \rho \leftrightarrow l \), and \( \kappa \leftrightarrow k \).
Appendix F

Miscellaneous Formulae

• We would like a function, call it $\Gamma(x)$, over $x \in \mathbb{R}$, such that it generalizes the notion of the factorial with: $\Gamma(n+1) = n!$ for $n \in \mathbb{N}_0$. Recall that the factorial is defined by the recurrence relation: $n! = n(n-1)!$ with $0! = 1$. Therefore, we want our “Gamma function” to obey its own defining recurrence relation: $\Gamma(x+1) = x \Gamma(x)$ with $\Gamma(1) = 1$. The following formula

$$\Gamma(x) = \int_0^\infty s^{x-1} e^{-s} ds$$ (F1)

solves the desired recurrence relation, which can easily be shown using integration by parts.

• The “generalized binomial coefficient” is defined via

$${a \choose b} = \frac{a(a-1)(a-2)\cdots(a-b+1)}{b(b-1)(b-2)\cdots1} \quad \text{or,} \quad {a \choose b} = \frac{\Gamma(a+1)}{\Gamma(b+1)\Gamma(a-b+1)}$$ (F2)

where $a$ is in a commutative ring and $b \in \mathbb{N}_0$ for the left equation, or $a, b \in \mathbb{R}$ for the right.

• The “(generalized) Laguerre polynomials,” $L^\alpha_\beta(x)$, are solutions to the ODE

$$x \frac{d^2y}{dx^2} + (\beta + 1 - x) \frac{dy}{dx} + \alpha y = 0$$ (F3)

• The “Bessel’s functions (of the first kind),” $J_n(x)$ are solutions to the ODE

$$x^2 \frac{d^2y}{dx^2} + x \frac{dy}{dx} + (x^2 - n^2) y = 0$$ (F4)

• The “spherical Bessel’s functions (of the first kind),” $j_n(x)$, are solutions to the ODE

$$x^2 \frac{d^2y}{dx^2} + 2x \frac{dy}{dx} + [x^2 - n(n+1)] y = 0$$ (F5)

• The “Whittaker functions (of the first kind),” $M_{a,b}(x)$ are solutions to the ODE

$$\frac{d^2y}{dx^2} + \left( \frac{1}{4} + \frac{a}{x} + \frac{\frac{1}{4} - b^2}{x^2} \right) y = 0$$ (F6)
Appendix F. Miscellaneous Formulae

- The “spherical harmonics,” \( Y_{lm}(\theta, \phi) \), are solutions to the PDE

\[
r^2 \nabla^2 Y_{lm}(\theta, \phi) = -l(l + 1) Y_{lm}(\theta, \phi)
\]

where we take the normalization such that: \( Y_{00} = 1/\sqrt{4\pi} \). Note that spherical harmonics are simultaneous eigenfunctions of the angular momentum operators \( \hat{L}_z \) and \( \hat{L}^2 \) via

\[
\hat{L}_z Y_{lm} = m Y_{lm} \quad \text{and} \quad \hat{L}^2 Y_{lm} = l(l + 1) Y_{lm} \tag{F7}
\]

- The reduced matrix elements of the spherical tensor form of a spherical harmonic, \( Y_{LM} \), are

\[
\langle l || \hat{Y}_L || l' \rangle = (-1)^L \frac{\hat{L} \, \hat{L}'}{\sqrt{4\pi}} \left( \begin{array}{cc} l & L \\ 0 & 0 \end{array} \right) \tag{F8}
\]

We may extend Equation (F8), using \( \hat{Y}_L = [\hat{Y}_L \otimes \mathbf{1}_0]_L \) and the analog of (B27) of Corollary B.2.4, to obtain the reduced matrix elements for a single spin-1/2 particle as [5]

\[
\langle l \frac{1}{2} j || \hat{Y}_L || l' \frac{1}{2} j' \rangle = (-1)^{L+j-j'} \frac{1}{2} + (-1)^{L+j'+j} \frac{\hat{L} \, \hat{L}'}{\sqrt{4\pi}} \left( \begin{array}{cc} j & j' \\ \frac{1}{2} & -\frac{1}{2} \end{array} \right) \tag{F9}
\]

- Consider a two-body spherical tensor operator, \( \hat{T} \) of rank 0, such that, in relative coordinates

\[
\langle n_r l_r || \hat{T} || n_{r'} l_{r'} \rangle \propto \delta_{n_r n_{r'}} \implies \langle l_1, l_2: L || \hat{T} || l_{1'} l_{2'}: L' \rangle = \delta_{L L'} \hat{L} \sum_{n_r l_r, N\Lambda} D_{12} D_{1'2'} \hat{L}^{-1} \langle n_r l_r || \hat{T} || n_{r'} l_{r'} \rangle \tag{F10}
\]

where \( D_{12} \equiv \langle n_r l_r, N\Lambda: L || n'_{1} l'_{1}, n'_{2} l'_{2}: L \rangle \) and \( D_{1'2'} \equiv \langle n_r l_r, N\Lambda: L || n'_{1} l'_{1}, n'_{2} l'_{2}: L \rangle \), and the CTML can be found in Equation (D13).

- For a substance with \( N_0 \) number of constituents, whereby it decays with a half-life of \( T_{1/2} \), then the substance obeys the exponential decay formula

\[
N(t) = N_0 e^{-\lambda t} \quad \text{where,} \quad \lambda = \frac{\ln(2)}{T_{1/2}} \tag{F11}
\]