WIGNER X RESOLVED AND PHOTO-REACTION CROSS-SECTION
PREDICTIONS: IMPROVEMENTS FOR ASTROPHYSICAL
CALCULATIONS

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by

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________________________

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Abstract
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Nuclear potential energy surfaces are generated using a micro-macro model. This is done in an automated procedure called AutoTAC which is used to find equilibrium deformation parameters corresponding to an energy minimum. This information will be used as a starting point for nuclear structure calculations with implications that are of astrophysical significance.

IBM $\zeta-\chi$ parameter fits based on energy ratios and transition probabilities are used to determine the ground state shape probability distribution from experimentally measured input. An alternative approach involves mapping fermionic potential energy surfaces on to bosonic space. This can predict the low-lying excitation spectrum as well as the probability distribution of the ground state. The probability distributions can be combined with the dipole strength function calculated using QRPA. The Instantaneous Shape Sampling (ISS) procedure involves adding many weighted strength functions, which is particularly important for the photo-absorption cross-section of transitional nuclei.

The linear coefficient in symmetry energy term of nuclei, called the Wigner X, is determined from the experimental binding energies by removing the Coulomb
energy by use of mirror nuclei with corrections for deformation based on additional experimental information. Energy differences are calculated using groups of three nuclei along an isobaric chain in steps of $\Delta T_z = 2$, starting at $N \simeq Z$. The resulting energy dependence is of the form $T(T + X)$ and appears to involve fluctuations about $X = 1$ and $X = 4$. For the strong pairing limit of isovector pairing the dependence should be of the form $T(T + 1)$, which reflects the spontaneous breaking of the isorotational symmetry by the isovector pair field. Correlations generated by the isovector monopole pairing interaction are treated exactly by means of diagonalization for small 6 and 7 level systems. The equilibrium deformation parameters calculated in AutoTAC are used as input.

The Wigner X observable is particularly sensitive to the deformation. In mid-shell regions, theoretically determined deformations are fairly constant and small, whereas experimental values are large and varied. In closed shell regions, where the theoretical deformations appear to be more accurate, the model excellently reproduces the observable. It is shown that allowing for slight adjustments of the experimentally determined deformation parameters will reproduce the large amplitude fluctuations seen experimentally for $A \approx 80$. The pairing calculations also allow for comparisons with the energy difference between the even-even and odd-odd mass parabolas to be determined, using the same procedure. The results indicate that the same pairing mechanisms that mediate the pairing gap are also responsible for the Wigner X.
For my friends and family.
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CHAPTER 1

INTRODUCTION

1.1 Motivation

This work is a building block to help answer the most fundamental of questions about the origin of the elements. Network nucleosynthesis calculations simulate the physics of stellar events and allow for the calculation of observed abundances of nuclei in the Universe. These have two major inputs: cross-sections for a reaction to occur and the masses of the nuclei involved. This thesis attempts to provide improvements for both of the inputs.

Cross-sections of nuclear reactions near the Gamow window are usually too low energetically to be measured experimentally. This is because it is very difficult to reproduce some astrophysical environments in a controlled laboratory setting. The low lying levels provide a great amount of additional information about the structure of a nucleus, which can be combined with the dipole strength function, providing insight into low energy photo-absorption/disintegration, important to processes in element synthesis.

1.2 Astrophysics

By the late 1950’s, a fairly complete picture of the processes involved in nucleosynthesis had been proposed [21]. The landscape of nuclear astrophysics is
summarized in Figure 1.1. These processes are described in detail in Appendix D, providing an explanation of how the elements in Table 1.1 are created.

Modern nucleosynthesis calculations use the Hauser–Feshbach theory which is based on the statistical model for reaction cross-sections. The cross-sections and the nuclear binding energies are combined with our knowledge of astrophysical environments, resulting in the predicted chemical abundances. Theoretical advancements in such simulations provide insight into which nuclear properties are of greatest importance [97].

A reliable prediction of the photo-absorption probability is important, specifically $(\gamma, n), (\gamma, p), (\gamma, \alpha)$ as well as the inverse $(n, \gamma), (p, \gamma), (\alpha, \gamma)$ reactions. Little is known about these reactions when they occur far from stability in the r-process and rp-process.

In addition, the masses or the directly related binding energies of nuclei near $N = Z$ have long been observed to contain some phenomena occurring which, until this work, was not well understood. Accurate binding energies of $N \approx Z$ nuclei are also extremely important for astrophysical phenomena such as the rp-process.

The mean field techniques described in this work are applicable for nuclei larger than $^{16}O$. From an astrophysical perspective, they are particularly relevant to the explosive elements synthesis of heavy nuclei.

1.3 Nuclear Structure

In addition to being relevant for improving our understanding of astrophysics, the two specific questions addressed here are particularly interesting from the nuclear structure point of view. This text will focus on nuclear structure. The two topics are generally unrelated, but the tools developed for the cross-section
Figure 1.1. The nuclear landscape showing stable elements and a few of the process paths on which the heaviest elements were created. The gray squares indicate nuclei from the Audi Mass Evaluation [5] with experimentally measured binding energies. The black squares denote nuclei that are stable according to Krane [72].
TABLE 1.1

THE NATURAL ABUNDANCES OF THE ELEMENTS IN THE SOLAR SYSTEM [91]

<table>
<thead>
<tr>
<th>Element</th>
<th>Mass Fraction</th>
<th>Number Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^1$H</td>
<td>0.71</td>
<td>0.94</td>
</tr>
<tr>
<td>$^4$He</td>
<td>0.27</td>
<td>0.06</td>
</tr>
<tr>
<td>$^6$Li, $^8$Be, $^{10}$B</td>
<td>$10^{-8}$</td>
<td>$10^{-9}$</td>
</tr>
<tr>
<td>$^{12}$C, $^{14}$N, $^{16}$O, $^{20}$Ne</td>
<td>$1.8 \times 10^{-2}$</td>
<td>$10^{-3}$</td>
</tr>
<tr>
<td>Si Group: $^{22}$Na, ..., $^{44}$Ti</td>
<td>$2 \times 10^{-3}$</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>Fe Group: $50&lt;A&lt;62$</td>
<td>$2 \times 10^{-4}$</td>
<td>$4 \times 10^{-6}$</td>
</tr>
<tr>
<td>Intermediate Mass: $63&lt;A&lt;100$</td>
<td>$10^{-6}$</td>
<td>$10^{-8}$</td>
</tr>
<tr>
<td>Heavy Mass: $A&gt;101$</td>
<td>$10^{-7}$</td>
<td>$10^{-9}$</td>
</tr>
</tbody>
</table>
calculations, particularly the AutoTAC deformations, are also important and are used as the starting point for the Wigner X calculation.

The Wigner X problem is the existence of a term proportional to $|N - Z|$ in the symmetry energy in nuclear binding energy. Most nuclear mass models just adjust a coefficient of proportionality of this term and avoid questioning its origin [30], [81], [29]. It has long been believed to be related to pairing; however depending on which formalism is used, the results will vary. In the strong pairing limit, conjectures based on SU(2) and supermultiplet algebras imply that the observed quantity would be $X = 1$ or $X = 4$ respectively. Experimentally, the average of these is seen as $X \approx 2.5$ [127]. In Chapter 6 it is shown that isovector pairing used with a moderate pairing strength on single particle levels can explain the experimental X values.

Another interesting phenomena is shape coexistence in nuclei. The energy spectra from the excited states of some nuclei, for example, $^{98}$Mo, contain a secondary low lying rotational band with $E(0^+_2) < 1$ MeV [103]. This is a characteristic of shape coexistence where this second band is a ground state band built around a secondary potential energy minimum. In addition, all nuclei fluctuate around their equilibrium shape or various shapes in cases with shape coexistence.

Long standing techniques exist that allow for the calculation of the photo-reaction cross-sections, but these take into account only the equilibrium deformation in a static approximation. In Chapter 4 a framework to account for shape fluctuations based on an adiabatic approximation is discussed. The use of the Interacting Boson Approximation facilitates the calculation of a probability distribution for the different shapes, and cross-sections can be calculated.
1.4 Outline of Thesis

The format of the Chapters 2-6 will be identical. The first section will describe the problem that is addressed in the Chapter and provide a very general background. The second section provides an in depth background. The third section describes the new work and highlights the results.

Chapter 2 covers some general theoretical background, particularly of material used in Tilted Axis Cranking (TAC) calculations and of the creation of an automated version called AutoTAC. Chapter 3 addresses the mapping of a mean field fermionic potential onto a bosonic Hamiltonian, which allows for the calculation of shape fluctuations. Chapter 4 discusses the development of the Instantaneous Shape Sampling (ISS) procedure and its application in calculating the dipole absorption strength functions for transitional nuclei. Chapter 5 describes an experimental analysis of various terms relating to the binding energy, in particular the Wigner X, which will be compared with theoretical calculations. Chapter 6 demonstrates how the Wigner X is generated by the isovector pairing interaction, and this is compared to the results from Chapter 5.

Chapter 7 summarizes the results. The appendices contain supplemental information. Appendix A presents additional background information on pairing approaches. Appendix B discusses new pairing approaches that have been developed but were not applied to a specific topic. Appendix C contains two approaches developed to determine the probability distribution for the ground state of nuclei. Appendix D discusses astrophysical processes relevant to this material. Appendix E shows some of the notes that were used in various calculations.
2.1 Introduction to the Shell Model

Mendeleev’s periodic table of elements grouped atoms in such a way that characteristic chemical behavior was classified and predicted for elements that were unknown at the time. The explanation was later provided in terms of the quantized orbitals in the electrons of an atom.

The periodicity as seen in atomic orbitals is also seen in nuclei. It is understood to be the result of the shell structure of nuclei [116]. Table 2.1 contains the magic numbers for which nuclei are particularly stable in terms of the proton number ($Z$) and the neutron number ($N$). The table compares the magic numbers from experimental evidence and the oscillator prediction of shell closure by Nilsson’s Modified Harmonic Oscillator model.

2.1.1 Wood-Saxon (WS)

There is, however, one crucial difference between the atomic orbitals for electrons and the nuclear levels for protons and neutrons. The major contributor to atomic orbitals is the central Coulomb potential created by the protons in the nucleus. The electron cloud shields this primary field as a secondary effect. For the nucleons, there is no external field, and therefore, a nucleon moves in a po-
potential created by all the other nucleons. As a consequence of the short range of the nucleon-nucleon interaction, on the order of femtometers \( \text{fm} = 10^{-15} \text{m} \), this potential is attractive. It is well represented by the Wood-Saxon profile:

\[
V = -V_0 f(r).
\]  

(2.1)

Where, \( f(r) \) is the Fermi distribution depending on the radial coordinate, defined as:

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

(2.2)

\( V_0 \) is the potential depth. \( R \) is the radius of the nucleus and \( a \) is related to the diffuseness of the nuclear surface. This potential is shown in Figure 2.1. The radius depends on the atomic mass number \( A = N + Z \), such that:

\[
R = R_0 A^{1/3}.
\]  

(2.3)

The WS potential gives a good description of the Coulomb barrier which is important in charged particle reactions. The barrier is caused by the electrostatic force, making two like sign charges repel each other. This force falls off as \( \frac{1}{r^2} \), which means that at short distances, the force will become large. Nuclei are so small that the potential can stop charged particles from colliding even at very high speeds. Tunneling allows for the Coulomb barrier to be penetrated without having the classically required center of mass kinetic energy.

A deformed WS potential is widely used in nuclear models. It has the same
<table>
<thead>
<tr>
<th>Shell</th>
<th>Electrons</th>
<th>Protons</th>
<th>Neutrons</th>
<th>Nilsson</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
<td>8</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>28</td>
<td>20</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>4</td>
<td>36</td>
<td>28</td>
<td>28</td>
<td>28</td>
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<td>5</td>
<td>54</td>
<td>50</td>
<td>50</td>
<td>50</td>
</tr>
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<td>6</td>
<td>86</td>
<td>82</td>
<td>82</td>
<td>82</td>
</tr>
<tr>
<td>7</td>
<td>118</td>
<td>126</td>
<td>126</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>186</td>
<td></td>
<td></td>
<td>184</td>
</tr>
</tbody>
</table>
Figure 2.1. The Fermi distribution $f(r)$ provides a good approximation to the density of nucleons in a nucleus. A WS potential, dominated by the short range strong force, is used to describe the potential generated by the strong interaction between nucleons. The Coulomb potential of a charged sphere is used to approximate the repulsive Coulomb interaction between the protons.
form as (2.1), but the radius has a directional dependence, such that:

\[
R = R_0 \left( 1 + \beta_2 \cos(\gamma) Y_{20}(\theta, \phi) + \beta_2 \frac{\sin(\gamma)}{\sqrt{2}} \left( Y_{22}(\theta, \phi) + Y_{2-2}(\theta, \phi) \right) \right). \tag{2.4}
\]

The spherical harmonics \( (Y_{2\mu}) \) are expressed in terms of the polar coordinates \((\theta, \phi)\). The deformation parameter \( \beta_2 \) determines the deviation from a spherical shape. The deformation parameter \( \gamma \) determines the deviation from an axial shape. For \( \gamma = 0 \) the nucleus has a prolate shape, and for \( \gamma = \frac{\pi}{3} \) the nucleus has an oblate shape. A more detailed discussion is given in Section 2.2.2.

Generally, the results based on the WS, relevant to the material described in this thesis, are quite comparable to the results of the Modified Harmonic Oscillator described next.

2.1.2 Modified Harmonic Oscillator (MHO) Model

An alternative approach begins with a spherical Harmonic Oscillator (HO) potential, which reproduces the magic numbers of the lowest shells but diverges with experimental data after the first few shells. The addition of a strong spin-orbit term is able to reconcile the difference \[54\].

The MHO used by Nilsson includes a spin-orbit term and an \( \vec{l}^2 \) term. It can be formalized in such a way as to account for deformation \[90\]. This is done with:

\[
H_{MHO} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{M}{2} \left( \omega_{\perp}^2 (x^2 + y^2) + \omega_z^2 z^2 \right) - 2\kappa \hbar \omega_0 \left( \vec{l} \cdot \vec{s} \right) - \kappa_\mu \hbar \omega_0 \left( \vec{l}^2 - \left\langle \vec{l}^2 \right\rangle_N \right). \tag{2.5}
\]
TABLE 2.2


<table>
<thead>
<tr>
<th>N</th>
<th>$\kappa_p$</th>
<th>$\mu_p$</th>
<th>$\kappa_n$</th>
<th>$\mu_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.120</td>
<td>0.00</td>
<td>0.120</td>
<td>0.00</td>
</tr>
<tr>
<td>1</td>
<td>0.120</td>
<td>0.00</td>
<td>0.120</td>
<td>0.00</td>
</tr>
<tr>
<td>2</td>
<td>0.105</td>
<td>0.00</td>
<td>0.105</td>
<td>0.00</td>
</tr>
<tr>
<td>3</td>
<td>0.090</td>
<td>0.30</td>
<td>0.090</td>
<td>0.25</td>
</tr>
<tr>
<td>4</td>
<td>0.065</td>
<td>0.57</td>
<td>0.070</td>
<td>0.39</td>
</tr>
<tr>
<td>5</td>
<td>0.060</td>
<td>0.65</td>
<td>0.062</td>
<td>0.43</td>
</tr>
<tr>
<td>6</td>
<td>0.054</td>
<td>0.69</td>
<td>0.062</td>
<td>0.34</td>
</tr>
<tr>
<td>7+</td>
<td>0.054</td>
<td>0.69</td>
<td>0.062</td>
<td>0.26</td>
</tr>
</tbody>
</table>

The inclusion of the $\vec{l}^2 - \langle \vec{l}^2 \rangle$ term simulates the correct radial profile, similar to the WS potential. The oscillator frequency is determined as a function of $A$, with:

$$h\omega_0 = 41A^{-1/3}[MeV].$$ (2.6)

The dimensionless parameters $\kappa$ and $\mu$ determine the strengths of the $\vec{l} \cdot \vec{s}$ and $\vec{l}^2$ terms. The parameters will change depending on the oscillator shell number (N). These have been fit using the energy spectra of spherical nuclei near doubly magic numbers for neutrons and protons [11]. The resulting values are in Table 2.2 which leads to Figure 2.2 for the neutron energy levels.
Figure 2.2. Nilsson neutron single particle energies as a function of deformation ($\varepsilon_2$). For spherical nuclei, with $\varepsilon_2 = 0$, large level gaps are seen at magic numbers. For non-spherical deformation, the magnetic moment quantum number degeneracy is broken and level splitting occurs. Generated by Jie Sun using TAC code.
The oscillator frequencies are stretched as a function of deformation, such that:

\[ \omega_{x,y,z} = \omega_0(\varepsilon_2, \gamma) \left( 1 - \frac{2}{3} \varepsilon_2 \cos \left( \gamma - \frac{2\pi n}{3} \right) \right). \]  

(2.7)

The index \( n \) is used such that \( n = 1 \) is used for \( \omega_x \), 2 for \( \omega_y \) and 3 for \( \omega_z \). The conservation of volume condition is fulfilled by adjusting \( \omega_0(\varepsilon_2, \gamma) \), so that the following is true:

\[ \omega_x \omega_y \omega_z = \omega_0^3(\varepsilon_2, \gamma) \prod_{n=1}^{3} \left( 1 - \frac{2}{3} \varepsilon_2 \cos \left( \gamma - \frac{2\pi n}{3} \right) \right) = \omega_0^3(\varepsilon_2 = 0, \gamma = 0). \]  

(2.8)

The deformation parameters \( \varepsilon_2 \) and \( \beta_2 \) are closely related as will be discussed later.

2.2 The Nuclear Mean Field

The assumption that nucleons move independently in an average potential is the most fundamental approximation in solving the many body problem of interacting nucleons. The many body interaction of a nucleon with all others is replaced by a one body potential created by the surrounding nucleons. The Hartree-Fock (HF) method is used to determine the average potential, the wavefunctions, and single particle energies of the individual nucleons. The method assumes that the many body state is well approximated by an anti-symmetrized Slater determinant \[56\] \[39\]. This is written as:

\[ |HF\rangle = \prod_{i=1}^{A} \hat{a}_i^\dagger |0\rangle. \]  

(2.9)
Here, $\hat{a}_i^+$ is the fermionic creation operator on a vacuum state $|0\rangle$ in which no particles exist. This creation operator obeys the following fermionic commutation relations in second quantized form:

$$
\left[ \hat{a}_i, \hat{a}_j^+ \right]_+ = \hat{a}_i \hat{a}_j^+ + \hat{a}_j^+ \hat{a}_i = \delta_{ij},
$$

(2.10)

and

$$
\left[ \hat{a}_i, \hat{a}_j \right]_+ = \left[ \hat{a}_i^+, \hat{a}_j^+ \right]_+ = 0.
$$

(2.11)

The energy expectation value of the many body HF wave-function is reduced to a field comprised of all averaged two body interactions [98]. This is expressed as:

$$
E_{HF} = \langle HF | H | HF \rangle = \sum_{i=1}^{A} \epsilon_i - \frac{1}{2} \sum_{ij=1}^{A} \bar{v}_{ijij}.
$$

(2.12)

The one body potential problem in the coordinate space is a Schrödinger equation, of the form:

$$
-\frac{\hbar^2}{2m} \nabla^2 \varphi_i(\vec{r}) + \sum_{j=1}^{A} \int d\vec{r}' v(\vec{r}, \vec{r}') \varphi_j(\vec{r}')^* \left( \varphi_j(\vec{r}') \varphi_i(\vec{r}) - \varphi_j(\vec{r}) \varphi_i(\vec{r}') \right) = \epsilon_i \varphi_i(\vec{r}).
$$

(2.13)

The problem is solved by iteration. The wave-functions can be assumed and the eigenvalue problem is solved. Then, assuming the corrections to the Hamiltonian based on the previous result, the wave-functions $(\varphi_i(\vec{r}))$ can be calculated.
This is repeated until the solutions converge. Single particle wave-functions and energies \( \epsilon_i \) then result. The WS potential and Nilsson can be thought of as good approximations of the HF method.

2.2.1 Tilted Axis Cranking (TAC)

The Tilted Axis Cranking approach was developed to describe the rotational properties of nuclei [42], [40]. The Hamiltonian of the cranking model represents the energy of a deformed nucleus in a coordinate system that rotates with an angular velocity \( \vec{\omega} \) [65], [16]. The single particle Schrödinger equation in the rotating frame is derived from the Routhian \( H' \), the Hamiltonian in the rotating frame, by means of the mean field approximation discussed previously, written as:

\[
H' = H - \hbar \vec{\omega} \cdot \vec{J}. \tag{2.14}
\]

In this thesis, the TAC model and the pertinent computer code are mainly applied to non-rotating nuclei. The rotational capabilities are only used to calculate the energy of the \( 2^+_1 \) state, \( E(2^+_1) \), which is used to set the total energy scale of the IBM mapping fits discussed in Chapter 3. Therefore, there will be no further discussion of the rotational aspects of the TAC model.

Instead of solving the HF equations, the TAC uses the micro-macro method, also called the shell correction method or Strutinsky method.

The total energy is the sum of the energy of a Deformed Liquid Drop with some charge \( Q = Ze \), the shell corrections \( E_{\text{shell}} \) which are calculated from the Wood-Saxon or Nilsson Levels, and the pairing energy, such that:

\[
E_{\text{total}} = E_{\text{DLD}} + E_{\text{shell}} + E_{\text{pair}}. \tag{2.15}
\]
All of these terms depend on the deformation parameters.

2.2.2 Deformation Parameters

Nuclei can deform as a result of competition between the surface energy, Coulomb repulsion, and pairing effects. However, shell structure plays the most important role in driving the nucleus to a shape for which high level density, near the Fermi energy, is avoided. The shapes considered here will be ellipsoidal with at most 3 unequal axes and some higher order hexadecapole deformations.

As a starting point, the definition of deformation parameters assumes that two of the principal axes are equal. With this, one can define a quadrupole deformation parameter ($\beta_2$), as:

$$\beta_2 = \frac{4}{3} \sqrt{\frac{\pi}{5}} \frac{\Delta R}{R_{\text{Avg}}}.$$  \hspace{1cm} (2.16)

$\Delta R$ is the difference between the semi-major and semi-minor axes of the ellipsoid. An oblate shape is defined when the two equal axes are larger than the remaining axis ($\beta_2 < 0$). A prolate shape is one in which the lone axis is larger than two equal axes ($\beta_2 > 0$). If $\beta_2 = 0$ then the shape is spherical.

Experimental $B(E2)$ transition probabilities are used to infer the quadrupole moment and the $\beta_2$ deformation parameter [96]. This is the source of all experimental deformations used in this text with the following conversion:

$$|\beta_2| = \left( \frac{4\pi}{3Z R_0^2} \frac{B(E2)}{e^2} \right)^{1/2}.$$  \hspace{1cm} (2.17)

The $B(E2)$ is the reduced electric quadrupole transition rate from the $0^+$ ground state to the excited $2^+$ state of even-even nuclei in units of ($e^2b^2$). $R_0$ is the mean radius of nuclear matter with $R_0^2 = 0.0144A^{2/3}b$.  

17
Triaxial shapes are also possible. Although they occur less frequently than the axial shapes, oblate and prolate, they play an important role in transitional nuclei. These are described by (2.4). Energies are usually displayed on a pie wedge as in Figure 2.3, where $\beta_2$ is the radial coordinate and $\gamma$ is the angle.

More general shapes include the hexadecapole deformation denoted by $\beta_4$. The scattering of nuclei with $\alpha$ particles indicates that the hexadecapole distortions are important in rare earth and actinide regions [80].

In this case, the radius as a function of polar angles is slightly modified:

$$R = R_0 \left(1 + \beta_2 Y_{20}(\theta, \phi) + \beta_4 Y_{40}(\theta, \phi)\right).$$  \hspace{1cm} (2.18)

The elongation distortion parameter ($\varepsilon_2$) and the hexadecapole distortion parameter ($\varepsilon_4$) are the natural variables for calculations with MHO Hamiltonian. The general characteristics of these parameters are shown in Figure 2.4.

One can transform between the two sets of parameters, $\beta_{2,4}$ and $\varepsilon_{2,4}$ using (2.19)-(2.21). Where $\beta_2$ is defined in the following way:

$$\beta_2 = \sqrt{\frac{\pi}{5}} \left(\frac{4}{3} \varepsilon_2 + \frac{4}{9} \varepsilon_2^2 + \frac{4}{27} \varepsilon_2^3 + \ldots\right).$$ \hspace{1cm} (2.19)

The inverse approximations apply for intermediate deformations with $-0.2 \lesssim \beta_2 \lesssim 0.4$ and $-0.05 \lesssim \beta_4 \lesssim 0.15$ [10]. They are the following:

$$\varepsilon_2 \approx 0.944\beta_2 - 0.122\beta_2^2 + 0.154\beta_2\beta_4 - 0.199\beta_4^2,$$ \hspace{1cm} (2.20)

and

$$\varepsilon_4 \approx -0.852\beta_4 + 0.141\beta_4^2 + 0.122\beta_2\beta_4 + 0.295\beta_2^2.$$ \hspace{1cm} (2.21)
Figure 2.3. Potential energy surfaces for some molybdenum isotopes built using Nilsson Levels with the pairing $\Delta$ defined in [2.38] and [2.39]. The AutoTAC minimum $\varepsilon_4$ is used and the remaining parameters $\varepsilon_2$ and $\gamma$ are plotted. The low lying energy spectrum of $^{98}$Mo contains characteristic $E(0^+_2) = 734.75 \pm 0.04$ keV [118] of shape coexistence not seen in this potential because pairing has effectively smoothed it out.
Figure 2.4. Depiction of the shapes described by the deformation parameters $\varepsilon_2$ and $\varepsilon_4$ [91]. Increasing $\varepsilon_2$ will make a shape less plate-like and more cigar-like, while increasing $\varepsilon_4$ will make a shape less lemon-like and more box-like. Generated by Mathew Meixner using the LightWave 3D software.
2.2.3 Deformed Liquid Drop (DLD) Energy

The macroscopic DLD terms are from an advanced form of the original Bethe-Weisäcker formula described in detail in Section 5.1.2, which takes the deformation dependence into account:

\[
E_{DLD} = -a_v A \left(1 - k_v \left(\frac{N-Z}{A}\right)^2\right) + \frac{3}{5} \frac{e^2 Z^2}{4 \pi \epsilon_0 R_0} \left(B_c(\beta_2, \gamma) - \frac{5 \pi^2}{6} \left(\frac{d}{R_0}\right)^2\right) + a_s A^{2/3} \left(1 - k_s \left(\frac{N-Z}{A}\right)^2\right) B_s(\beta_2, \gamma). \quad (2.22)
\]

The coefficients, \(a_v = 15.494\) MeV, \(a_s = 17.944\) MeV, \(k_v = k_s = 1.783\), \(d = 0.544\) fm and here \(R_0 = 1.225A^{1/3}\) fm, have been modified from [84] and differ slightly from what is used in Chapter 5 for spherical binding energies.

The term \(B_c\) is the ratio of the Coulomb energy of a charged deformed ellipsoid to the Coulomb energy of a charged sphere of the same volume [57]. This is written as:

\[
B_c(\beta_2, \gamma) = 1 - \frac{\beta_2^2}{4 \pi} - \frac{1}{105} \left(\frac{5}{4 \pi}\right)^{3/2} \beta_2^3 \cos(3\gamma). \quad (2.23)
\]

The term \(B_s\) is the ratio of the surface area of a deformed ellipsoid to the surface area of a sphere of the same volume, written as:

\[
B_s(\beta_2, \gamma) = 1 + \frac{\beta_2^2}{2 \pi} - \frac{2}{21} \left(\frac{5}{4 \pi}\right)^{3/2} \beta_2^3 \cos(3\gamma). \quad (2.24)
\]
2.2.4 Strutinsky Energy Corrections

The shell energy is the difference between the sum of the single particle energies calculated from the MHO or WS potentials and a smooth energy, such that:

\[ E_{\text{shell}} = 2 \sum_i \epsilon_i - 2 E_{\text{smooth}}. \] (2.25)

The smooth energy is derived from the single particle levels by means of Strutinsky’s averaging procedure \[113], \[85]. This defines the smooth energy as:

\[ E_{\text{smooth}} = \int_{-\infty}^{\lambda} \epsilon \bar{g}(\epsilon) d\epsilon. \] (2.26)

The average level density (\(\bar{g}(\epsilon)\)) uses the discrete levels and a smearing function which depends on the parameter \(\Gamma\), such that:

\[ \bar{g}(\epsilon) = \frac{1}{\Gamma \sqrt{\pi}} \sum_i f \left( \frac{\epsilon - \epsilon_i}{\Gamma} \right) e^{-\left( \frac{\epsilon - \epsilon_i}{\Gamma} \right)^2}. \] (2.27)

The \(f(u)\) is a special function comprised of Hermite polynomials \(H_n(u)\), written as:

\[ f(u) = \sum_{k=0}^{n} \frac{(-1)^k}{(2k)!!2^k} H_{2k}(u). \] (2.28)

The whole procedure is done in such a way that \(\bar{g}(\epsilon)\) depends smoothly on \(\epsilon\), reproducing the global change of the level density.

The smoothed Fermi energy (\(\tilde{\lambda}\)) is determined by the condition for the number of particles, with:

\[ \mathcal{N} = 2 \int_0^{\tilde{\lambda}} \bar{g}(\epsilon) d\epsilon. \] (2.29)
2.2.5 Monopole Pairing with Quasi-particles

The Bardeen, Cooper, and Schrieffer (BCS) method that accounts for pairing in nuclei was originally used to describe superconductivity \[8\]. It will be covered in detail in Appendix A and only the basics will be presented here. When pairing is included in a calculation, the single particle energies are replaced by quasi-particle energies using the Bogoliubov quasi-particle transformation \[14\].

The operators $\hat{\alpha}_i^+$ and $\hat{\alpha}_i^-$ that create quasi-particles are defined by the following transformation. They also obey the fermionic commutation relations:

$$\hat{\alpha}_i^+ = u_i \hat{a}_i^+ - v_i \hat{a}_i^-, \quad (2.30)$$

and

$$\hat{\alpha}_i^- = u_i \hat{a}_i^- + v_i \hat{a}_i^+. \quad (2.31)$$

The amplitudes $u_i$ and $v_i$ are real. The occupation probability ($v_i^2$) of the single particle levels are as follows:

$$v_i^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_i - \lambda}{\tilde{\epsilon}_i} \right), \quad (2.32)$$

and

$$u_i^2 = \frac{1}{2} \left( 1 + \frac{\epsilon_i - \lambda}{\tilde{\epsilon}_i} \right). \quad (2.33)$$

The quasi-particle energies ($\tilde{\epsilon}_i$) are defined in the following way:

$$\tilde{\epsilon}_i = \sqrt{(\epsilon_i - \lambda)^2 + \Delta^2}. \quad (2.34)$$
The pairing energy will now be a function of both the pairing gap ($\Delta$) and the chemical potential ($\lambda$). The minimization with respect to the pairing gap, gives the self consistency equation:

$$
\Delta = G \sum_i u_i v_i. \quad (2.35)
$$

The chemical potential is introduced in such a way that the average particle number ($\mathcal{N}$) is correct, with:

$$
\mathcal{N} = 2 \sum_i v_i^2. \quad (2.36)
$$

(2.35) and (2.36) are coupled and solved for protons and neutrons separately. The details of this procedure are described in Appendix E.1. The total energy gain due to the pairing correlations ($E_{\text{pair}}$) is the following result:

$$
E_{\text{pair}} = 2 \sum_i \epsilon_i \left( v_i^2(\Delta, \lambda) - v_i^2(\Delta = 0, \lambda) \right) - \frac{\Delta^2}{G}. \quad (2.37)
$$

2.3 AutoTAC

Möller and Nix et al. have published equilibrium deformations calculated by means of a micro-macro method using a folded Yukawa single particle potential [81]. The model was later improved to also allow for triaxiality [82]. The extended calculations of the equilibrium deformations and binding energies of several thousand nuclei produced a few hundred nuclei which appear to be triaxial. This is done by calculating the binding energy, as in (2.15), for various shapes and finding which combination of deformation parameters corresponds to the energy minimum.
The theoretical results in the following chapters are based on the TAC mean field. In all cases, information related to the equilibrium deformation is a necessity. For this reason, the equilibrium deformations of the MHO and WS potential were calculated for the whole nuclear chart. Thus, an automated version of the TAC was created and used, called AutoTAC.

The pairing effects are calculated using standard BCS pairing based on the phenomenological fits by Möller and Nix \cite{79}. The fits used are the following:

\[ \Delta_{pBCS} = \frac{13.4}{A^{1/2}}[MeV], \]  

(2.38)

and

\[ \Delta_{nBCS} = \frac{12.8}{A^{1/2}}[MeV]. \]  

(2.39)

The ground state deformation is determined by means of an automated minimization program that was built on the existing TAC code with no rotation. All AutoTAC calculations discussed in this text will represent the ground state deformation with the above pairing. For that reason, the major distinction between TAC and AutoTAC is that AutoTAC was used to find the equilibrium deformations and potential energy surfaces only. The term TAC implies the use of a more general code that also calculates wave-functions, \( B(E2) \) values, rotational properties, and more.

Two dimensional potential energy surface are minimized in AutoTAC. Volume is conserved, and single particle occupation configurations are traced on the grid. AutoTAC used alternating grids and found the minimum deformation parameters \( \varepsilon_2, \varepsilon_4 \) and \( \gamma \). Odd iterations involve the \( \varepsilon_2 - \gamma \) grid. Even iterations are in the \( \varepsilon_4 - \gamma \) plane. This procedure was chosen because of the relatively slowly changing
behavior of the triaxial parameter.

Coarse grids were used in the beginning and were enhanced after each of the first eight iterations. Iterations are continued beyond the 8th until the deformation parameters converge. AutoTAC was used for 3500+ even-even nuclei and took approximately 5 computer-months to complete for both Wood-Saxon and Nilsson runs. The resulting deformation parameters are generally consistent with the results of Möller and Nix.

The resulting table of deformation parameters certainly has its limitations. There is no information about how soft a potential is or if there is a secondary minimum. This is the case of the transitional nuclei which will be discussed in Chapter 4. This can make illustrations like, Figure 2.8, a bit misleading, because it seems as if the different models have completely different oblate to prolate shapes, while in reality the full potential contains both minima in delicate balance. Fortunately, it is very simple to quickly generate the potential using the table as a starting point, on a case by case basis. These potentials are used as the starting point in the mapping technique that will be discussed in Chapter 3.

The AutoTAC deformation parameter results are available on the internet at:

www.nd.edu/~ibentley/AutoTAC.xls
Figure 2.5. Quadrupole deformation parameter $\varepsilon_2$ from the Möller and Nix data set. Deformation is small near magic numbers, and well deformed cases generally peak at the furthest points from magic numbers.
Figure 2.6. Quadrupole deformation parameter $\varepsilon_2$ from the AutoTAC Wood-Saxon calculation. The results are quite comparable with those of Möller and Nix. The range of nuclei for which this calculation was performed is greater than that of the previous work.
Figure 2.7. Quadrupole deformation parameter $\varepsilon_2$ from the AutoTAC Nilsson calculation. The results are also quite comparable with those of Möller and Nix. Interesting physics may be occurring in regions where there are significant discrepancies.
Figure 2.8. Comparison of $|\varepsilon_2|$ deformation parameter for molybdenum isotopes resulting from experimental $B(E2)$ converted from Raman et al. 2001 data, calculations by Möller and Nix, and AutoTAC results for a Wood-Saxon and Nilsson levels.
Figure 2.9. Comparison of $|\varepsilon_2|$ deformation parameter for tin isotopes resulting from experimental $B(E2)$ converted from Raman et al. 2001 data, calculations by Möller and Nix, and AutoTAC results for a Wood-Saxon and Nilsson levels.
CHAPTER 3
CALCULATIONS OF THE PARAMETERS OF THE INTERACTING BOSON
MODEL BY MAPPING FROM FERMIONIC POTENTIAL ENERGY
SURFACES

3.1 Motivation and the Interacting Boson Model (IBM)

For the calculations of the photo-absorption cross-sections of transitional nu-
clei, which will be discussed in Chapter 4, a description of the fluctuations of
the nuclear shape for the ground state is needed. The IBM Hamiltonian contains
parameters that are used to determine the dynamics of the nuclear shape. Typi-
cally, these parameters are determined by a fit to the energies and electromagnetic
transition rates of the lowest collective states, as will be discussed in Section 4.3.1.

However, for many nuclei in astrophysical network calculations this informa-
tion does not exist. Therefore, there is a need to calculate the parameters of the
IBM model by purely theoretical means. This chapter explores one possible ap-
proach. It should be pointed out that calculation of the IBM parameters from the
fermionic structure has been a challenge since the advent of the IBM, which has
many other applications that that are not addressed in this thesis.

The IBM is based on the approximation that pairs of nucleons behave like
bosons with either angular momentum 0 or 2 \[2\]. Creation operators for the two
spins are denoted by \(s^+\) and \(d^+\) respectively \[64\]. This provides a description of
quadrupole states in even-even nuclei in terms of the SU(6) group [4]. The IBM-1 formalism, in which protons and neutrons are indistinguishable is a powerful tool for predicting the low lying energy spectra based on a simple Hamiltonian [108], [135]. A simple version of the IBM Hamiltonian is used that is sufficient [120]. This is written as a function of two IBM parameters, such that:

\[ H_{IBM}(\zeta, \chi) = c \left( (1 - \zeta) \hat{n}_d - \frac{\zeta}{4N_B} \hat{Q}^x \cdot \hat{Q}^x \right), \]

(3.1)

with

\[ \hat{n}_d = d^+ \cdot \tilde{d}, \]

(3.2)

and

\[ \hat{Q}^x = (s^+ \tilde{d} + d^+ s) + \chi (d^+ d)^2. \]

(3.3)

The parameters \( \zeta \) and \( \chi \) then define a triangle with in which most nuclei can be placed [23]. The U(5) vibrational limit occurs when \( \zeta = 0 \) and well describes a spherical nucleus. The O(6) \( \gamma \)-soft limit has \( \zeta = 1 \) and \( \chi = 0 \), representing nuclei that have no rigidity in the triaxial degree of freedom. The SU(3) oblate or prolate rotor limit is when \( \zeta = 1 \) and \( \chi = \sqrt{7/2} \) or \( \chi = -\sqrt{7/2} \) respectively.

3.2 Mapping of Fermionic to Bosonic Potential Energy Surfaces

Micro-macro mean field methods allow for the calculation of the energy as a function of the deformation parameters, \( \beta_2 \) and \( \gamma \), which is called the Potential Energy Surface (PES). The expectation values of the IBM Hamiltonian with a coherent state, \( |N, \beta_B, \gamma_B \rangle \) can be used to create IBM PES [49], [120]. The
state is comprised as a product of boson creation operators ($\hat{B}^+$), with:

$$|N\beta_B\gamma_B\rangle = \frac{1}{\sqrt{N!}} \hat{B}^N|0\rangle,$$

(3.4)

and

$$\hat{B}^+ = s^+ + \beta_B \left( \cos(\gamma_B)d_0^+ + \frac{\sin(\gamma_B)}{\sqrt{2}}(d_2^+ + d_{-2}^+) \right).$$

(3.5)

The basic idea suggested by Nomura et al. is to match the fermionic PES ($E_{MF}(\beta, \gamma)$) with the bosonic PES ($E_{IBM}(\beta_B, \gamma_B)$) [94]. This mapping fixes the parameters of (3.1), which are then used to calculate the low-lying collective states. The expectation value of the IBM Hamiltonian is the following:

$$E_{IBM}(\beta_B, \gamma_B) = \langle N\beta_B\gamma_B\mid H_{IBM} \mid N\beta_B\gamma_B \rangle$$

$$= c_E \left[ \frac{(1-\zeta)N_B(\beta_B)^2}{1+(\beta_B)^2} - \left( \frac{\zeta(N_B-1)(\beta_B)^2}{(1+(\beta_B)^2)^2} \right) \right] \times \left( 1 - \sqrt{\frac{2}{7}} \chi \beta_B \cos(3\gamma_B) + \frac{N^2}{14}(\beta_B)^2 \right).$$

(3.6)

The assumption that the deformations of the protons and neutrons are approximately equal justifies the use of an IBM-1 based Hamiltonian [18], [77], $N_B$ is the number of bosons. Conventionally, this is taken to be half the number of valence nucleons.

The bosonic deformation parameters are related to the mean field deformation parameters by:

$$\gamma_B = \gamma, \text{ and } \beta_B = c_\beta \beta_2.$$  

(3.7)

Success using this technique has been shown and it has been used to predict the low-lying energy spectrum for various nuclear shapes [94]. However, a priori
knowledge was used in setting parameters to be consistent with previous fits. One example of the use of prior knowledge is the setting of the $\chi$ for the protons to be a constant. The work of Nomura et al. was performed using the IBM-2 formalism which allows for protons and neutrons to be treated separately [94]. This choice of parameters reduced the procedure to the IBM-1 formalism. The previous work has a shortcoming resulting from the use of Skyrme Hartree-Fock with BCS pairing. These potential energy surfaces have fluctuations which do not allow for automated fitting. This approach seems to have involved fits of the potential energy surfaces to be done by looking for the optical likeness between potentials.

There are four unknowns including two scaling coefficients. The $c_E$ is the total energy scale, and $c_\beta$ sets the deformation scale, which will be defined as the global IBM parameters. According to Nomura et al. range for the deformation scale parameter is $2 \lesssim c_\beta \lesssim 7$ [94].

The local IBM parameters are the remaining unknowns $\zeta$ and $\chi$. Energy ratios can be used so the scaling parameter $c_E$ drops out. Therefore, the two parameters, $\zeta$ and $\chi$, define the energy ratios [77]. The ratios of interest are the following:

$$R_{4/2} = \frac{E(4^+_1)}{E(2^+_1)},$$ (3.8)

$$R_{\beta/2} = \frac{E(0^+_2)}{E(2^+_1)},$$ (3.9)

and

$$R_{\gamma/2} = \frac{E(2^+_2)}{E(2^+_1)}.$$(3.10)
The last two are referred to as the $\beta$-band and $\gamma$-band head ratios.

In Section 4.3.1, a method is described in which experimental levels are used to determine $\zeta$ and $\chi$. Table 3.1 contains the parameters for some gadolinium and erbium isotopes derived from the experimental energies.

3.3 AutoTAC to IBM Mapping

TAC is used to create the PES, $E_{TAC}(\beta_2, \gamma, \omega = 0)$. The hexadecapole contribution that is calculated in the AutoTAC is held constant. This mapping procedure, which deviates from that of Nomura et al., minimizes the mean squared deviations ($d^2$) between $E_{TAC}(\beta_2, \gamma)$ and $E_{IBM}(\beta_B, \gamma_B)$, with:

$$d^2(\zeta, \chi, c_\beta) = \sum_i \left( E_{TAC}(\beta_i, \gamma_i, \omega = 0) - E_{IBM}(\beta_i, \gamma_i, N_B = 10, \zeta, \chi, c_\beta) \right)^2. \quad (3.11)$$

Both potentials are set equal to zero at the minimum corresponding to the equilibrium deformation. The number of bosons was set to $N_B = 10$ for all nuclei. The main purpose of using a fixed number of bosons is that it can be applied within the framework of the ISS described in the next chapter.

The TAC PES don’t have the same fluctuations as the Skyrme based PES of Nomura et al. allowing them to be fit with an automated procedure. Another significant improvement from the previous IBM mapping work is that the total energy scale, $c_E(\zeta, \chi)$, coefficient is determined in a different way. Taking advantage of the capabilities of TAC code, the $E(2^+_1)$ is calculated. It is found by minimizing the $E_{TAC}(\beta_2, \gamma, I(\omega) = 2)$. Frauendorf et al. have calculated the $E(2^+_1)$ for the Pd and Cd isotopes used later [44]. J. Sun calculated the energies for the remaining
TABLE 3.1

IBM PARAMETERS FROM MCCUTCHAN ET AL. [77].

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Number of Bosons</th>
<th>ζ</th>
<th>χ</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{152}$Gd</td>
<td>10</td>
<td>0.41</td>
<td>-1.32</td>
</tr>
<tr>
<td>$^{154}$Gd</td>
<td>11</td>
<td>0.59</td>
<td>-1.10</td>
</tr>
<tr>
<td>$^{156}$Gd</td>
<td>12</td>
<td>0.72</td>
<td>-0.86</td>
</tr>
<tr>
<td>$^{158}$Gd</td>
<td>13</td>
<td>0.75</td>
<td>-0.80</td>
</tr>
<tr>
<td>$^{160}$Gd</td>
<td>14</td>
<td>0.84</td>
<td>-0.53</td>
</tr>
<tr>
<td>$^{162}$Gd</td>
<td>15</td>
<td>0.98</td>
<td>-0.30</td>
</tr>
<tr>
<td>$^{156}$Er</td>
<td>12</td>
<td>0.55</td>
<td>-0.62</td>
</tr>
<tr>
<td>$^{158}$Er</td>
<td>13</td>
<td>0.63</td>
<td>-0.61</td>
</tr>
<tr>
<td>$^{160}$Er</td>
<td>14</td>
<td>0.69</td>
<td>-0.60</td>
</tr>
<tr>
<td>$^{162}$Er</td>
<td>15</td>
<td>0.75</td>
<td>-0.53</td>
</tr>
<tr>
<td>$^{164}$Er</td>
<td>16</td>
<td>0.84</td>
<td>-0.37</td>
</tr>
<tr>
<td>$^{166}$Er</td>
<td>17</td>
<td>0.91</td>
<td>-0.31</td>
</tr>
<tr>
<td>$^{168}$Er</td>
<td>18</td>
<td>0.82</td>
<td>-0.36</td>
</tr>
</tbody>
</table>
nuclei, specifically the Mo, Gd and Er isotopes. This energy is defined as:

\[ E(2^+_1)_{TAC} = E_{TAC}(I(\omega) = 2) - E_{TAC}(I(\omega) = 0). \]  

The ratio of the \( E(2^+_1) \) energies determines the energy scale, with:

\[ c_E(\zeta, \chi) = \frac{E(2^+_1)_{TAC}}{E(2^+_1)_{IBM}(\zeta, \chi)}. \]  

The other three parameters are varied until the IBM potential best reproduces the AutoTAC potential below a 100 keV energy cutoff. This choice of matching area has a drawback that can be seen in Figures 3.7 and 3.10. The sharp upturn of the AutoTAC potential of well deformed nuclei is not reproduced in the IBM potential. However, this choice does seem to best reproduce the profile of the PES with respect to the triaxial parameter. The results of this procedure are shown in Tables 3.2 and 3.3.

Using a higher energy cutoff on the order of 1 MeV generally finds the beta deformation with a better accuracy but at the expense of getting a less accurate gamma deformation. The resulting levels are not in good agreement when compared to experiment.

The energies and ratios of the \( B(E2) \) transition probabilities of low-lyings collective states are calculated by diagonalizing \( H_{IBM}(c_E, \chi, \zeta) \) using the parameters determined by the mapping procedure.

Excellent agreement with experiment is obtained for the cadmium and palladium isotopes of both the energy levels and transition strengths, as seen in Figures 3.2, 3.4 and 3.13. Every step of the procedure appears to have been successful. The curvature of the TAC PES is well reproduced by the IBM PES and the TAC PES seem to provide a good representation of the nuclei. The only discrepancy
for these comparisons is existence of an intruder state, making the theoretical the \( \beta \)-band head appear to be too high in energy, which is a limitation of the IBM.

For the molybdenum nuclei, shown in Figure 3.5, the gamma softness is generally well reproduced, while the exact triaxial minimum is unattainable using this simple Hamiltonian. Again, the theoretical the \( \beta \)-band head appear to be too high in energy. This has been attributed to being a result of shape coexistence. The use of a secondary IBM calculation can eliminate this 101.

In the case of the gadolinium and erbium isotopes, there appears to be some problem. In Figures 3.7 and 3.10, an additional PES comparison is included using the \( \zeta \), \( \chi \) and \( N_B \) from energy ratio fits by McCutchan et al. 77. A mean value of \( c_\beta = 4.5 \) is used for the purpose of plotting. This comparison gives insight to the interplay of the various parameters, for which the experimental levels are in better agreement with an IBM calculation using roughly the same \( \zeta \) but a drastically different value \( \chi \). The PES do not contain this information. There is the additional problem that the curvature of the TAC PES for well deformed nuclei cannot be generated using such a simple IBM Hamiltonian.

For these nuclei, the effect on the low-lying levels of scaling the energy based on the experimental \( E(2^+_1) \), as opposed to TAC, is shown in Figures 3.8, 3.9, 3.11 and 3.12. Basically, this indicates that there are a few cases where the small discrepancy of the TAC \( E(2^+_1) \) is to blame for disagreement with the experimental levels.

Overall, this approach appears to work well for nuclei with small to moderate deformations, and would need no further development for predictive calculations of the low lying energy spectra of similar nuclei that are of astrophysical importance.
<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Energy Scale</th>
<th>Deformation Scale</th>
<th>$\zeta$</th>
<th>$\chi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{108}$Cd</td>
<td>2.52</td>
<td>3.5</td>
<td>0.54</td>
<td>-0.52</td>
</tr>
<tr>
<td>$^{110}$Cd</td>
<td>2.69</td>
<td>3.0</td>
<td>0.54</td>
<td>-0.48</td>
</tr>
<tr>
<td>$^{112}$Cd</td>
<td>2.20</td>
<td>3.0</td>
<td>0.56</td>
<td>-0.10</td>
</tr>
<tr>
<td>$^{114}$Cd</td>
<td>2.05</td>
<td>3.5</td>
<td>0.60</td>
<td>0.24</td>
</tr>
<tr>
<td>$^{116}$Cd</td>
<td>2.26</td>
<td>4.0</td>
<td>0.64</td>
<td>0.10</td>
</tr>
<tr>
<td>$^{102}$Pd</td>
<td>2.28</td>
<td>4.0</td>
<td>0.54</td>
<td>-0.78</td>
</tr>
<tr>
<td>$^{104}$Pd</td>
<td>2.31</td>
<td>4.0</td>
<td>0.60</td>
<td>-0.52</td>
</tr>
<tr>
<td>$^{106}$Pd</td>
<td>2.21</td>
<td>4.0</td>
<td>0.66</td>
<td>-0.26</td>
</tr>
<tr>
<td>$^{108}$Pd</td>
<td>2.08</td>
<td>4.0</td>
<td>0.72</td>
<td>-0.14</td>
</tr>
<tr>
<td>$^{110}$Pd</td>
<td>1.97</td>
<td>4.0</td>
<td>0.78</td>
<td>-0.12</td>
</tr>
<tr>
<td>$^{112}$Pd</td>
<td>2.29</td>
<td>4.5</td>
<td>0.86</td>
<td>-0.14</td>
</tr>
<tr>
<td>$^{98}$Mo</td>
<td>2.04</td>
<td>3.5</td>
<td>0.64</td>
<td>-0.06</td>
</tr>
<tr>
<td>$^{100}$Mo</td>
<td>2.75</td>
<td>3.5</td>
<td>0.72</td>
<td>-0.02</td>
</tr>
<tr>
<td>$^{102}$Mo</td>
<td>2.66</td>
<td>3.0</td>
<td>0.74</td>
<td>0.02</td>
</tr>
<tr>
<td>$^{104}$Mo</td>
<td>2.15</td>
<td>3.0</td>
<td>0.80</td>
<td>0.02</td>
</tr>
<tr>
<td>$^{106}$Mo</td>
<td>1.73</td>
<td>3.0</td>
<td>0.80</td>
<td>0.02</td>
</tr>
<tr>
<td>$^{108}$Mo</td>
<td>1.77</td>
<td>3.0</td>
<td>0.66</td>
<td>0.66</td>
</tr>
</tbody>
</table>
**TABLE 3.3**

ADDITIONAL IBM PARAMETERS FROM FITTING OF AUTOTAC POTENTIAL ENERGY SURFACES WITH 10 BOSONS.

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Energy Scale</th>
<th>Deformation Scale</th>
<th>( \zeta )</th>
<th>( \chi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{150}\text{Gd})</td>
<td>1.91</td>
<td>4.5</td>
<td>0.64</td>
<td>-0.24</td>
</tr>
<tr>
<td>(^{152}\text{Gd})</td>
<td>2.63</td>
<td>6.0</td>
<td>0.98</td>
<td>-0.14</td>
</tr>
<tr>
<td>(^{154}\text{Gd})</td>
<td>2.14</td>
<td>5.0</td>
<td>0.94</td>
<td>-0.32</td>
</tr>
<tr>
<td>(^{156}\text{Gd})</td>
<td>1.49</td>
<td>3.5</td>
<td>0.64</td>
<td>-1.12</td>
</tr>
<tr>
<td>(^{158}\text{Gd})</td>
<td>1.55</td>
<td>4.5</td>
<td>0.92</td>
<td>-0.38</td>
</tr>
<tr>
<td>(^{160}\text{Gd})</td>
<td>1.63</td>
<td>4.0</td>
<td>0.90</td>
<td>-0.60</td>
</tr>
<tr>
<td>(^{162}\text{Gd})</td>
<td>1.46</td>
<td>3.5</td>
<td>0.70</td>
<td>-1.16</td>
</tr>
<tr>
<td>(^{156}\text{Er})</td>
<td>1.65</td>
<td>4.0</td>
<td>0.66</td>
<td>-0.54</td>
</tr>
<tr>
<td>(^{158}\text{Er})</td>
<td>1.51</td>
<td>4.0</td>
<td>0.68</td>
<td>-0.64</td>
</tr>
<tr>
<td>(^{160}\text{Er})</td>
<td>1.54</td>
<td>3.5</td>
<td>0.70</td>
<td>-0.80</td>
</tr>
<tr>
<td>(^{162}\text{Er})</td>
<td>1.84</td>
<td>4.5</td>
<td>1.00</td>
<td>-0.38</td>
</tr>
<tr>
<td>(^{164}\text{Er})</td>
<td>1.39</td>
<td>3.5</td>
<td>0.66</td>
<td>-1.16</td>
</tr>
<tr>
<td>(^{166}\text{Er})</td>
<td>1.69</td>
<td>4.0</td>
<td>0.96</td>
<td>-0.58</td>
</tr>
<tr>
<td>(^{168}\text{Er})</td>
<td>1.71</td>
<td>4.0</td>
<td>0.86</td>
<td>-1.00</td>
</tr>
</tbody>
</table>
Figure 3.1. IBM mapping potential comparisons for cadmium nuclei. In general these are very well reproduced by the IBM.
Figure 3.2. IBM mapping low lying levels prediction for cadmium nuclei compared with experiment, with good agreement of the respective band heads and the $E(4^+_1)$. The black lines indicate the experimental levels and the red lines indicate the results using this mapping technique.
Figure 3.3. IBM mapping potential comparisons for palladium nuclei. The IBM potential is not sophisticated enough to reproduce the secondary oblate minimum of $^{112}$Pd.
Figure 3.4. IBM mapping low lying levels prediction for palladium nuclei compared with experiment. A secondary minimum may explain the low lying $E(0^+_2)$ in the later palladium.
Figure 3.5. IBM mapping potential comparisons for transitional molybdenum nuclei.
Figure 3.6. IBM mapping low lying levels prediction for molybdenum nuclei compared with experiment. Again the very low lying $E(0^+_2)$ is an indication of shape coexistence. In these cases an alternative approach is necessary.
Figure 3.7. IBM mapping potential comparisons for gadolinium nuclei. The third column includes the IBM potential energy surfaces based on the $\zeta$ and $\chi$ created by the fitting by McCutchan et al., using the number of valence bosons. A constant $c_\beta = 4.5$ is assumed.
Figure 3.8. IBM mapping low lying levels prediction for gadolinium nuclei compared with experiment. The gray levels indicate what the $\zeta$ and $\chi$ fits by McCutchan et al. would generate. The pink levels indicate the same result but the TAC $E(2^+_1)$ is used instead of the experimental $E(2^+_1)$. Note that for $^{150}$Gd there is no comparison with the previous $\zeta$-$\chi$ fit.
Figure 3.9. Additional IBM mapping low lying levels prediction for gadolinium nuclei compared with experiment.
Figure 3.10. IBM mapping potential comparisons for erbium nuclei. Again the third column includes the IBM potential energy surfaces based on the $\zeta$ and $\chi$ created by the fitting by McCutchan et al., using the number of valence bosons and a constant $c_\beta = 4.5$. 
Figure 3.11. IBM mapping low lying levels prediction for erbium nuclei compared with experiment. The gray levels indicate what the $\zeta$ and $\chi$ fits by McCutchan et al. would generate. The pink levels indicate the same result but the TAC $E(2^+_1)$ is used instead of the experimental $E(2^+_1)$. 
Figure 3.12. Additional IBM mapping low lying levels prediction for erbium nuclei compared with experiment.
Figure 3.13. The $B(E2)$ transition probabilities from the TAC to IBM fits for $^{106}$Pd, $^{108}$Pd, $^{112}$Cd, and $^{156}$Gd compared to experimental measurements from [114], [73], [3]. The IBM probabilities are scaled to the experimental $B(E2, 2^+_1 \rightarrow 0^+_1)$ value. Note that the $^{156}$Gd transition probabilities are predominately out of band, resulting in small transition strengths.
CHAPTER 4

ELECTROMAGNETIC DIPOLE ABSORPTION IN TRANSITIONAL NUCLEI

4.1 Nuclear Reactions in Astrophysical Environments

The cross-section is a critical input in the simulation of astrophysical processes driven by nuclear reactions. The specific topic that is addressed in this text is the calculation of the photo-absorption cross-section of transitional nuclei. In astrophysical environments the photons are most commonly generated in charged particle reactions.

4.1.1 Reaction Energy Window

The reaction cross-section ($\sigma$) quantifies the consequences of nuclear properties on the probability of a reaction to occur. The reaction rate per unit volume ($R_V$) is the product of the cross-section with the number densities of the two reactants ($n_1$ and $n_2$) and their relative velocity ($v_{12}$), is defined as:

$$R_V(E) = \sigma(E)n_1(E)n_2(E)v_{12}(E).$$

Nuclear reactions are more likely to occur when the density and temperature are higher. The kinetic energy of particles at a certain temperature $T$ is given
by a Maxwell-Boltzmann distribution $n(E)$, the value of which decreases rapidly with the energy, such that:

$$n(E) \propto e^{-E/kT}. \quad (4.2)$$

The velocity will increase with the energy, with:

$$v(E) \propto \sqrt{E}. \quad (4.3)$$

For charge neutral elastic scattering the cross-section is constant. The cross-section of a low energy uncharged particle will decrease sharply as a function of energy for exothermic reactions [111]. For endothermic charged particle reactions, the Coulomb barrier penetration cross-section grows exponentially as a function of energy, such that:

$$\sigma(E) \propto \frac{1}{E} e^{-c\alpha/\sqrt{E}}. \quad (4.4)$$

The probability for the reaction to occur is only substantial where these distributions overlap. The overlap region is referred to as the Gamow window, which is illustrated in Figure 4.1. It is a range of energies in which charged particle reactions are most likely to occur in astrophysical environments. This thesis is concerned with $(p,\gamma)$ and $(\alpha,\gamma)$ reactions that involve the emission of a photon after the absorption of a proton or $\alpha$-particle. The Gamow window is located a few MeV above the reaction threshold. The threshold is equal to the reaction $Q$ value, with:

$$Q = \sum B_{E_{\text{reactants}}} - \sum B_{E_{\text{products}}}. \quad (4.5)$$
Figure 4.1. The Gamow peak of the reaction probability occurs when the high energy tail of the Maxwell-Boltzmann distribution $n(E)$ overlaps with the likelihood of tunneling through the Coulomb barrier $\sigma(E)$. 

\[ n(E) \nu(E) = C_1 E^{1/2} e^{-E/kT} \]

\[ \sigma(E) = C_2 e^{-C_3 \sqrt{E/E}} \]

\[ P(E) = n(E) \nu(E) \sigma(E) \]
The \((n,\gamma)\) and \((\gamma,n)\) reactions which involve the absorption of a neutron and the emission of a photon or the inverse, respectively, also play an important role in astrophysical reaction networks. These occur in the vicinity of the neutron binding energy. Yet another important reaction type is \((\gamma,p)\), which occurs at energies somewhat above the proton binding energy, such that the Coulomb barrier can be penetrated.

In the astrophysical network calculations a statistical theory of nuclear reactions is applied, where the \((\gamma,\text{ particle})\) reaction cross-section is the product of \(\sigma_\gamma\), the cross-section for the absorption of a photon, with the probability to emit the particle from the excited nucleus \[58\]. Hence, one needs the photo-absorption cross-section at the energy where the reaction takes place. This cross-section is proportional to the dipole strength function \(S(E)\), which is the transition probability from the ground state to all states within the energy interval \([E, E + dE]\).

According to the statistical theory, the cross-section for the inverse, \((\text{particle, } \gamma)\) reaction is given by the product of the particle absorption cross-section with the probability of emitting a photon from the excited nucleus. The latter is also directly related to the strength function. In the following, the calculations of the strength function or photo-absorption cross-section, which is equivalent, are considered.

4.1.2 Giant Dipole Resonance (GDR)

The GDR is a classic example of a collective excitation \[83\]. This resonance was discovered in studies of the photo-absorption of Uranium \[6\]. Even before this discovery, it was realized that a mean excitation frequency could be derived from nuclear polarizability \[78\]. The polarizability is a quantity related to the
symmetry energy in the mass formula which indicates the roles of protons and neutrons in the resonance. The relative distributions of protons and neutrons is the foundation for the conventional views of the resonance.

The Goldhaber-Teller description of the collective motion consists of proton and neutron fluids within spherical boundaries, which are displaced with respect to each other [51]. The Steinwedel-Jensen mode also is built on relative motion of the protons and neutrons, but in this case, it is internal density fluctuations that cause the resonance [112].

The GDR is generally peaked in an energy region from 10 to 25 MeV [18]. The resonance is observed as a broad Lorentzian distribution. The Lorentzian response function is the classical solution to a damped driven harmonic oscillator, where the width Γ is determined by the strength of the damping.

For deformed nuclei, energy distribution is observed as the sum of two Lorentzians created by vibrations about the long and short principal axes. Transitional nuclei show GDR that are broader, which is caused by the superposition of various shapes.

Conventionally, the smooth Lorentzian functional dependence of the resonance cross-section is traced down to the energy region where the astrophysical reactions take place, which is an approximation in which no nuclear structure occurs [12]. The full expression for the cross-section in this region should include resonance phenomena that are caused by the single particle structure. This is achieved by calculating the electromagnetic strength function of the vibrating nuclear system by means of the Random Phase Approximation (RPA).
4.2 Quasi-particle Random Phase Approximation (QRPA) and Resulting Strength Functions

The RPA was originally introduced to describe collective oscillations of electrons in a plasma \[15\]. The RPA is based on a quasi-boson approximation where pairs of fermions are approximated as bosons \[98\]. The consequences of this approximation will be discussed in detail in Appendix A.2. In calculating the dipole strength function, the dipole quasi-bosons \(\hat{\beta}_\mu^+\) are comprised of pairs of BCS quasi-particles defined in (2.30). This formalism is called the Quasi-particle RPA. It is based on the following bosonic operators:

\[
\hat{\beta}_\mu^+ = \hat{\alpha}_j^+ \hat{\alpha}_k^+, \quad \text{and} \quad \hat{\beta}_\nu = \hat{\alpha}_l \hat{\alpha}_m.
\]  

These quasi-boson operators are assumed to obey the standard bosonic commutation relations:

\[
[\hat{\beta}_\mu, \hat{\beta}_\nu^+] = \beta_\mu \beta_\nu^+ - \beta_\nu^+ \beta_\mu = \delta_{\mu\nu},
\]  

(4.7)

and

\[
[\hat{\beta}_\mu, \hat{\beta}_\nu] = [\hat{\beta}_\mu^+, \hat{\beta}_\nu^+] = 0.
\]  

(4.8)

The double index over all \(j\) and \(k\) such that \(j < k\) and is abbreviated as \(\mu\), and for \(l\) and \(m\), with \(l < m\), as \(\nu\).

This is called the quasi-boson approximation, because carrying out the commutation in (4.7) with the original pairs of fermionic quasi-particles will result in additional terms, which are neglected.

The QRPA approach will give vibrational excitations for deformed nuclei re-
stricting the configuration mixing to the those consisting of only two quasi-particle excitations and ground state correlations. A separable Hamiltonian is used for the QRPA which uses an interaction described by the products of general multipole operators \((Q_{\mu,t})\). In the case of the dipole response, these will take the form of a dipole operators. The Hamiltonian contains the unperturbed two quasi-particle excitations which are coupled by a series of factorized residual interaction terms \([32]\). The Hamiltonian is written as:

\[
H_{RPA} = \sum_{\mu} E_{\mu} \hat{\beta}_{\mu}^+ \hat{\beta}_{\mu} - \frac{1}{2} \sum_{\mu,t} \kappa_{\mu,t} Q_{\mu,t}^2.
\] (4.9)

In this model, \(\kappa\) is the strength of the interaction and the subscript \(\mu\) denotes the type of transition, for example, dipole. The dipole transition operators are defined as being comprised as functions of the spherical harmonic oscillator such that \(\hat{T} = r^l Y^m_l\) where \(l = 1\). The subscript \(t\) indicates how to treat the protons and neutrons, either as an isovector combination or as an isoscalar combination. Specifically, the combination will involve using either \(\frac{1}{2}(Q_{\text{proton}} - Q_{\text{neutron}})\) or \(\frac{1}{2}(Q_{\text{proton}} + Q_{\text{neutron}})\), respectively.

The single particle energies have been replaced with quasi-particle energies because the pairing interaction has been taken into account. The vibrational states \(|\Omega_i\rangle\) are expanded in terms of two quasi-particle \((\hat{\beta}_{\mu}^+\) and two quasi-hole excitations \((\hat{\beta}_{\mu})\) \([33]\). This is done such that:

\[
|\Omega_i\rangle = \sum_{\mu} [r_i(\mu) \hat{\beta}_{\mu}^+ + s_i(\mu) \hat{\beta}_{\mu}] |0\rangle_{RPA}.
\] (4.10)

The quasi-particle excitation spectrum and the corresponding wave-functions are calculated in the TAC. The amplitudes \(r_i(\mu)\) and \(s_i(\mu)\) are defined by the the
vibrational state:

\[ D_\mu = \langle 0 | \hat{D}_\mu \hat{\beta}_\mu | 0 \rangle. \]  

(4.11)

\( B_i \) is the strength of a transition from the RPA vacuum to a vibrational state with energy \( E_i = \hbar \Omega_i \), with:

\[ B_i = \sum_\mu \left| D_\mu \left[ r_i(\mu) + s_i(\mu) \right] \right|^2. \]  

(4.12)

At the energies of interest, \( \sim 10 \text{ MeV} \), there are very many solutions \( \Omega_i \) per unit energy. Thus the strength function is introduced to describe the nuclear properties, defined as:

\[ S(E) = \sum_i B_i \frac{\Delta/2\pi}{(E - \hbar \Omega_i)^2 + (\Delta)^2}. \]  

(4.13)

It represents the sum of the strengths of all transitions within an energy interval defined by \( \Delta \), producing the transition strength density.

From the strength function, the absorption cross-section can be calculated as the following:

\[ \sigma(E) = \frac{16\pi^2}{3hc} \sum_i E_i B_i \frac{\Delta/2\pi}{(E - \hbar \Omega_i)^2 + (\Delta)^2}. \]  

(4.14)

The following approximate relation is reliable for small widths \( \Delta \), where:

\[ \sigma(E) \approx \frac{16\pi^2}{3hc} ES(E). \]  

(4.15)

Since the cross-section is described by means of a Lorentzian weight function it can be calculated in a direct way using the spectral function method [34]. The
procedure is done by means of contour integration which is performed numerically, without resorting to the amplitudes $r_i(\mu)$ and $s_i(\mu)$.

4.3 Folded QRPA Solution Applied to Transitional Nuclei

The QRPA calculations are carried out for a static nuclear shape described by the deformation parameters of Section 2.2.2. However, there are transitional nuclei which strongly fluctuate between multiple shapes. The following presents a method of calculating the photo-absorption cross-section for transitional nuclei using a folding procedure.

The idea behind the folded QRPA strength function is quite simple. The strength function can be calculated for a nucleus at any given deformation. The probability of being at a given deformation is calculated for a grid of deformation parameters. For each grid point, the probability is multiplied by the corresponding strength function. The contributions from all points are added together as:

$$\sigma_{\text{total}}(E) = \sum_n P_n(\varepsilon_2, \gamma)\sigma_n(E, \varepsilon_2, \gamma).$$ (4.16)

Finding the probability distribution ($P_n$) of the deformation parameters is not a trivial task. Three different approaches have been studied. The first combines TAC PES with a simple kinetic energy term that assumes a constant mass parameter. The mass parameter is adjusted to reproduce the experimental $E(2_1^+)$ and $B(E2, 2_1^+ \rightarrow 0_1^+)$. The values of the mass parameter depended on $Z$ and $N$ in an erratic way and the method was subsequently abandoned. The method is discussed in detail in Appendix C.1.

A more sophisticated approach which involves a single particle configuration based deformation hopping picture, is included in Appendix C.2. This consists

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of allowing each configuration to have its own minimum deformation as determined by the single particle levels. In this case, the pairing strength is used to determine the mixing of various states. Ultimately, the resulting transition probabilities did not agree well with experiment. In addition, excited \(0^+\) states were not reproduced. Therefore, this approach was also discarded.

The successful approach uses IBM parameter fits.

4.3.1 IBM \(\zeta-\chi\) fits

As stated in the previous chapter, three experimental energy ratios, (3.8)-(3.10), can be used to determine \(\zeta\) and \(\chi\).

There are two inherent problems in comparing the \(O_2^+, O_3^+, 2_2^+,\) and \(2_3^+\) energy levels from the IBM with the experiment. First, the IBM energy levels do not specify which levels are the \(\gamma\)-band or \(\beta\)-band heads. However, this can be rectified with the use of the IBM predicted \(B(E2)\) values which will provide additional information about which levels reside in the same band. The second problem results from the fact that in this model, the levels from different bands are often mixed. The \(B(E2)\) information is combined with a two level model in order to remove the mixing of the levels, such that:

\[
C_2 = \left( \frac{E(2_3^+) - E(2_2^+)}{2} \right) \left( \frac{B(E2)_{>3_2^+2^+}}{B(E2)_{<3_2^+2^+}} \right),
\]

(4.17)

and

\[
C_0 = \left( \frac{E(0_3^+) - E(0_2^+)}{2} \right) \left( \frac{B(E2)_{>2_0^+0^+}}{B(E2)_{<2_0^+0^+}} \right).
\]

(4.18)

\(C_X\) is the correction removed from the larger energy and added to the smaller energy, depending on the \(B(E2)\) ratio so that the modified energy \((E')\) comes
from \( E'(X_2^+) = E(X_2^+) + C_X \), and \( E'(X_3^+) = E(X_3^+) - C_X \). The correction is necessary for the IBM levels only. If two levels have the same \( B(E2) \) ratio, then they are both equally likely to be in a given band. For this reason, the correction will adjust the two levels so that the energies become equal. These corrections are generally less than a few hundred keV and only will only slightly shift the \( \zeta-\chi \) results.

Figure 4.2 illustrates the overdetermined problem with two parameters that need to be solved for and three energy ratios that can be combined to find the best results. When experimental information on only two of these ratios exists, fits can still be performed.

It should again be noted that typical IBM calculations use the number of bosons being defined as half the number of valence fermions. However, for deformed nuclei, the concept of valence nucleons, far separated from an inert core, becomes somewhat unclear. For this reason, we have again restricted these calculations to contain 10 bosons. This has the advantage of using the same smooth IBM ratio surfaces in the \( \zeta-\chi \) fits. Also, the new procedures involving the IBM that are discussed in this text, use carefully crafted automated fits. IBM calculations are commonly fit by carefully comparing the energy ratios or, as was described in the previous section, the potential energy surface. Because of this, these automated IBM energy ratio fits of \( \zeta \) and \( \chi \) are by no means standard. A sufficient number of bosons is needed in order to sample the probability distribution for the ground state shapes described in the next section.
Figure 4.2. IBM $\zeta$-$\chi$ fit for $^{156}$Gadolinium based on the three commonly used energy ratios and associated 5% error in shaded regions. Grey-black is $R_{4/2}$. Pink-red is $R_{3/2}$. Finally, cyan-blue is $R_{\gamma/2}$. Giving the optimal values of $\zeta = .75$ and $\chi = -.94$ for a calculation with 10 bosons. The results from McCutchan et al. determined the values to be $\zeta = .72$ and $\chi = -.86$ for a calculation with 12 bosons [77].
4.3.2 Instantaneous Shape Sampling

Instantaneous Shape Sampling (ISS) is the procedure of combining the microscopic QRPA with the phenomenological IBM used to calculate dynamic properties of nuclei [136]. The folding procedure discussed previously is based on the fact that the two modes involved occur at two distinct time scales. The shape fluctuations occur at the scale $\sim \hbar / 0.5\text{MeV}$, which is slow compared to the dipole oscillations. The faster dipole oscillations occur on the scale $\sim \hbar / 15\text{MeV}$.

The total cross-section $\sigma_\gamma(E)$ is obtained as the incoherent sum of instantaneous cross-sections combined with the probability distribution of each that is present in the ground state, with:

$$\sigma_\gamma(E) = \sum_n P(\beta_n, \gamma_n) \sigma(E, \beta_n, \gamma_n). \quad (4.19)$$

The collective quadrupole mode is described by IBM-1 [64]. The IBM Hamiltonian and the $B(E2)$ operators are given by McCutchan et al. [77]. The corresponding parameters of the model are listed in Table 4.1, where $e_B$ is the effective boson charge. In case of shape coexistence, two sets of parameters are listed with the respective proportion in the ground state given as a percentage.

A sufficiently flexible basis is created using the fixed boson number $N_B = 10$. The probability distribution $P(\beta_n, \gamma_n)$ is generated by means of the method suggested by Tonev et al. [115]. This involves using two scalar operators ($\hat{q}_2$, $\hat{q}_3$) which are formed by angular momentum coupling from the IBM quadrupole operators $\hat{Q}_\mu^\chi$, with:

$$\hat{q}_2 = [\hat{Q}_x \otimes \hat{Q}_x]_0, \quad \text{and} \quad \hat{q}_3 = [\hat{Q}_x \otimes [\hat{Q}_x \otimes \hat{Q}_x]]_2. \quad (4.20)$$
**TABLE 4.1**

IBM PARAMETERS AND EQUILIBRIUM DEFORMATION
PARAMETERS CALCULATED BY MEANS OF THE
MICRO-MACRO METHOD.

<table>
<thead>
<tr>
<th>(^{AX})</th>
<th>(\zeta)</th>
<th>(\chi)</th>
<th>(\epsilon_b)</th>
<th>(%)</th>
<th>(\beta)</th>
<th>(\gamma)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{88}\text{Sr})</td>
<td>0.0</td>
<td>-1.20</td>
<td>0.043</td>
<td>100</td>
<td>0.0</td>
<td>0°</td>
</tr>
<tr>
<td>(^{90}\text{Zr})</td>
<td>0.0</td>
<td>-1.20</td>
<td>0.013</td>
<td>64</td>
<td>0.0</td>
<td>0°</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.60</td>
<td>-0.31</td>
<td>0.040</td>
<td>36</td>
<td></td>
</tr>
<tr>
<td>(^{92}\text{Mo})</td>
<td>0.25</td>
<td>-1.32</td>
<td>0.040</td>
<td>100</td>
<td>0.0</td>
<td>0°</td>
</tr>
<tr>
<td>(^{94}\text{Mo})</td>
<td>0.29</td>
<td>-1.20</td>
<td>0.064</td>
<td>100</td>
<td>0.02</td>
<td>60°</td>
</tr>
<tr>
<td>(^{96}\text{Mo})</td>
<td>0.20</td>
<td>-1.32</td>
<td>0.069</td>
<td>100</td>
<td>0.10</td>
<td>60°</td>
</tr>
<tr>
<td>(^{98}\text{Mo})</td>
<td>0.0</td>
<td>-1.20</td>
<td>0.053</td>
<td>60</td>
<td>0.18</td>
<td>37°</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.59</td>
<td>-0.03</td>
<td>0.106</td>
<td>40</td>
<td></td>
</tr>
<tr>
<td>(^{100}\text{Mo})</td>
<td>0.0</td>
<td>-1.20</td>
<td>0.053</td>
<td>40</td>
<td>0.21</td>
<td>32°</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.61</td>
<td>-0.10</td>
<td>0.106</td>
<td>60</td>
<td></td>
</tr>
</tbody>
</table>
The commuting operators $\hat{q}_2$ and $\hat{q}_3$ are diagonalized in the space of states generated by coupling the bosons to zero angular momentum. The resulting eigenvalues ($q_{2,n}$ and $q_{3,n}$) and the eigenstates $|n\rangle$ are linked to the deformation parameters by the following expressions which assume that the charge density and the mean field have the same deformation, with:

$$\beta^2_n = \sqrt{5} \left( \frac{4\pi e_B}{3ZeR^2} \right)^2 q_{2,n}, \quad (4.21)$$

and

$$\cos 3\gamma_n = \sqrt{\frac{7}{2\sqrt{5}}} \frac{q_{3,n}}{(q_{2,n})^{3/2}}. \quad (4.22)$$

The probabilities $P(\beta_n, \gamma_n) = |\langle 0_1^+ | n \rangle|^2$ are the projections of the IBM ground state $|0_1^+\rangle$ on the set $|n\rangle$.

Some of the studied nuclei show shape coexistence where the low-lying $0_2^+$ state and the $0_1^+$ ground state are understood as mixtures of two different equilibrium shapes $a$ and $b$ with $c_a^2$ and $c_b^2 = 1 - c_a^2$ being the fractions of each shape in the ground state.

In this case, two families of states originate from the collective motion about the two different equilibrium shapes, which are described by two different sets of IBM parameters.

The different $c_a^2$ and $c_b^2$ and the experimental energies of the states $0_1^+$ and $0_2^+$ are used to calculate the energies of the pure states $0_a^+$ and $0_b^+$ and their interaction. Assuming the same interaction for the states $(1_1^+, 1_2^+, 2_1^+, 2_2^+, 4_1^+, 4_2^+)$, the energies and $B(E2)$ values of the pure states $2_a^+, 2_b^+, 4_a^+, 4_b^+$ are derived for which the IBM parameter sets $a$ and $b$ are fitted. The probability distributions $P(\beta_{n,a}, \gamma_{n,a})$ and $P(\beta_{n,b}, \gamma_{n,b})$ for each of the two IBM Hamiltonians are generated separately.
The probabilities for all instantaneous shapes of the ground state are $c^2_a P(\beta_{n,a}, \gamma_{n,a})$ and $c^2_b P(\beta_{n,b}, \gamma_{n,b})$. The sum in (4.19) is taken for all combinations.

The method is applied to the nuclei $^{88}$Sr, $^{90}$Zr and $^{92-100}$Mo. For these nuclei, earlier $(\gamma, n)$ measurement data are available on RIPL-2, which are combined with recent $(\gamma, \gamma')$ experiments at the ELBE facility, producing absorption cross-sections $\sigma_\gamma(E)$ covering the whole energy range from the GDR down to few MeV [9], [104], [105], [109], and [110]. The IBM parameters were obtained for each nuclei separately by fitting the energies and $B(E2)$ values of the lowest $0^+, 2^+, 4^+$ states taken from the ENSDF data base [118]. Besides the use of $N_B = 10$, the work of Garrett et al. and Cata et al. was followed, from which the fractions $c^2_a$ and $c^2_b$ of the coexisting shapes in $^{90}$Zr and $^{98,100}$Mo were taken [48], [24]. Figure 4.3 demonstrates that the resulting instantaneous shapes are widely distributed across the $\beta - \gamma$ plane, which reflects the transitional nature of the considered nuclei. In the cases of shape coexistence, the two sets of nearly spherical and well deformed shapes are clearly separated.

The coupling to excitations other than quadrupole becomes increasingly important as the energy increases. The $M1$-contribution to $\sigma_\gamma$ is about $5\%$, which is consistent with the scarce experimental information [109].

Transitional nuclei with ($Z = 38, 40, 42$, $N = 50$) and ($Z = 42$, $N = 52, 54, 56, 58$) are studied. ISS based on the QRPA very well reproduces the experimental photo-absorption cross-sections around the nucleon emission thresholds.

Folding with a Lorentzian of width $\Gamma = \alpha E^2$ is included, which depends on the photon energy $E$ as expected for collisional damping [125]. The coefficient $\alpha$ is chosen to reproduce the experimental $\sigma_\gamma$ at the maximum of the GDR, which gives $\alpha = 0.0105$ MeV$^{-1}$ for the neutron number $N = 50$ and 0.014 MeV$^{-1}$ for
Figure 4.3. IBM calculation ground state probability distribution for Molybdenum based on $\zeta$-$\chi$ fits used in the ISS calculations. Adapted from [136]
$N > 50$. This is done in order to account for other degrees of freedom which are not included in the calculation.

Figures 4.4, 4.5, and 4.6 compare the results with the experimental data. The figures show the absorption cross-section in the region near the nucleon emission thresholds. The blue dashed line indicates the cross-section for the equilibrium deformation as calculated in the QRPA. The red curve is the solution ISS with deformation based probability distribution multiplied by the corresponding QRPA solutions. The best procedure is shown in light green. This involves folding the ISS solution with a Lorentzian of width $\Gamma$ taking into account Collisional Damping (CD) in a phenomenological way. Effectively, the ISS is a model that takes into account the level structure, shape coexistence, and damping of the relative motion between the protons and neutrons.

The inclusion of CD in $\sigma_\gamma^{ISS-CD}$ smooths the fluctuations in the ISS-CD curves, but scarcely adds any dipole strength. Hence, the dipole strength near the nucleon emission threshold is determined by the Landau fragmentation of the instantaneous shapes, each of which contributes according to its ground state probability. While the resulting dipole strength deviates from a Lorentzian shape, it shows some of the underlying particle-hole structure.
Figure 4.4. The dipole absorption cross-section for $^{94}$Mo. The general shape of the resonance is best represented by the combined ISS-CD curve. Experimental data can be found in [105].
Figure 4.5. The cross-section for the ($\gamma$, $n$) reaction calculated with use of the ISS technique as a function of the neutron emission threshold of Molybdenum isotopes taken from [136]. $S_n = 9.68$, 9.15, 8.64 and 8.29 MeV for the isotopes with neutron number (N) = 52, 54, 56, and 58. Experimental data is a combination of a photon scattering experiment and ($\gamma$, $n$) reactions [124],[104].
Figure 4.6. The photo-disintegration cross-section for isotones with 50 neutrons calculated as a function of the mean of the proton and neutron thresholds taken from [136]. $(S_n + S_p)/2 = 10.86, 10.16$ and $10.06$ MeV for isotones with proton number $(Z) = 38, 40, 42$. Experimental data can be found in [109], [110].
CHAPTER 5

INVESTIGATION OF BINDING ENERGY TERMS

5.1 Nuclear Binding Energies

In Chapter 6, the Wigner X term in the symmetry energy of nuclei near \( N = Z \) is described as a consequence of isovector pairing. For a comparison with the experimental symmetry energy, all of the other energy components must be removed from the experimental binding energy. This can easily be done for all components but the Coulomb energy by taking the difference in binding energy along isobaric chains, where atomic mass number \( (A) \) is constant. Incrementing \( T_z \) in steps of 2 removes the even-odd mass parabola staggering. The symmetry and Coulomb energies both remain. The Coulomb energy is fit and removed, leaving just the symmetry energy and the observable of interest the Wigner X. In this chapter, the extraction procedure is described and the resulting values for the Wigner X are discussed.

5.1.1 Definition of Binding Energy

The binding energy is the amount of energy that holds a nucleus together. The binding energy is measured as being the difference in the mass of the sum of
component nucleons and electrons from the mass \( M \) of the nucleus, such that:

\[
B_E = [Z(m_p + m_e) + Nm_n - M]c^2.
\]  

(5.1)

The masses of the nucleons and nuclei can be measured with high precision, which allows for general characteristics to be investigated.

5.1.2 Bethe-Weizsäcker Mass Formula

The semi empirical mass formula, which is known as the Bethe-Weizsäcker formula, provides a basic insight into the mechanisms that determine the binding energy of a nucleus. It will be used to illustrate how to isolate and determine specific terms which can later be explained either from a classical or quantum mechanical viewpoint [123].

Although the Bethe-Weizsäcker formula certainly has its shortcomings, particularly missing nuclear deformation and shell effects, it is sufficient at describing global characteristics of the binding energies of nuclei with more protons and neutrons than \(^{16}\text{O}\). The various coefficients are from an empirical fit to experimental measurements of nuclear masses.

The Bethe-Weizsäcker formula has 5 terms accounting for the energy of a nucleus with a particular volume, surface area, charge, symmetry of neutrons and protons, and pairing of nucleons. The binding energy, as a function of the number of protons \( Z \) and neutrons \( N \) or related variables, is defined as:

\[
B_E = a_vA - a_sA^{2/3} - a_cZ(Z - 1)A^{-1/3} - a_{sym}A^{-1}|T_z|^2 \pm a_pA^{-1/2}.
\]  

(5.2)
Here the isospin projection $T_z$ is $|T_z| = \frac{1}{2}|N - Z|$. In Krane’s text, *Introductory Nuclear Physics*, the coefficients are $a_v=15.5 \text{ MeV}$, $a_s= 16.8 \text{ MeV}$, $a_c=.72 \text{ MeV}$, $a_{\text{sym}}=92 \text{ MeV}$, and $a_p = 34 \text{ MeV}$ [72]. It should be noted that the term of interest results from more in depth investigations where $|T_z|^2$ is replaced by $|T_z|(|T_z|+X)$.

5.1.3 Charged Liquid Droplet

The charged liquid drop model provides the justification for the first three terms in the Bethe-Weizsäcker formula. The nucleus is approximated as a drop of incompressible charged fluid. The first two terms come from arguments following analogies to the energy of a droplet of water. The nuclear force is short ranged. Therefore, one nucleon interacts only with its nearest neighboring nucleons, which is the same for all nucleons in the nuclear interior. This contributes the amount of binding energy that grows linearly with the total number of nucleons. Nuclear matter is nearly incompressible, so nuclear matter should have constant density. This implies that the volume is proportional to the atomic mass number ($A$), and the radius $R = r_0A^{1/3}$, with $r_0 \sim 1.2 fm$. A surface correction to the binding energy is included because nucleons on the surface have fewer nucleons near them. The number of nucleons on the surface is proportional to the surface area ($4\pi R^2 \propto A^{2/3}$).

The Coulomb term takes into account the fact that the nucleus contains positively charged protons which repel each other. To a good approximation, the nucleus can be treated as a charged sphere. Classically, a uniformly charged sphere has an energy that depends on its radius and the charge ($Q = eZ$), such
Figure 5.1. The binding energy per nucleon for all experimentally measured nuclei from the Audi Mass Evaluation [5]. The red line is an adjusted fit motivated by the Bethe-Weizsäcker formula. The binding energy is peaked around $A = 56 - 62$, which implies that these nuclei are the most tightly bound.
Figure 5.2. The binding energy per nucleon for all experimentally measured nuclei from the Audi Mass Evaluation compared to the Bethe-Weizsäcker formula. Significant deviations occur near magic numbers indicating the existence of shell structure.
that:

\[ E_C = \frac{3}{5} \frac{Q^2}{4\pi\epsilon_0 R}. \quad (5.3) \]

The relationship between the radius and atomic mass number can be used. Also, a factor of \( Z(Z - 1) \) is used, instead of just the quadratic term, because the charge is quantized, and charged protons will not repel themselves, giving the following relation:

\[ E_C = -B_C = \frac{3}{5} \frac{e^2}{4\pi\epsilon_0 r_0} Z(Z - 1)A^{-1/3}. \quad (5.4) \]

This can be written in terms of \( a_c \) from (5.2), where:

\[ E_C = a_c Z(Z - 1)A^{-1/3}. \quad (5.5) \]

5.2 Detailed Discussion of the Terms in the Mass Formula

Mirror nuclei can be used to single out the Coulomb energy, because they have the same value of \( |T_z| \). Historically, mirror nuclei have also been used to calculate the equivalent radius of a nucleus. Uncertainties in Coulomb fits are inherent, because most fits do not take into account the effects of deformation, or shell effects. The symmetry energy can be evaluated after the Coulomb energy is removed.

5.2.1 Historic Coulomb Fits

A comparison of phenomenological Coulomb fits with 149 experimentally measured differences in Coulomb energy has been carried out by Jänecke et al. [67].
The previous Coulomb fits compare well with more recent evaluations. The results A-E are included in Figures 5.8 and 5.9 and labeled as historic fit A-E. The quantity $\Delta E_C$ is the difference in Coulomb energy divided by difference in $Z$, which can be related to the partial derivative of the Coulomb energy by following expression:

$$\Delta E_C = \frac{\Delta E}{\Delta Z} \approx \frac{\partial E}{\partial Z} \bigg|_{Z=\bar{Z}}. \quad (5.6)$$

For mirror nuclei, $\Delta E_C$ is simply the difference in binding energy. From this information, the Coulomb energy ($E_C$) can be derived.

In general, the historic fits have the same leading order terms as (5.3), but with different corrections depending on the physics included. Historic Fit A includes an exchange term correction caused by the anti-symmetrization of wave-functions required to satisfy the Pauli exclusion principle. This is also the motivation behind the second term of the Myer Swiatecki (MS) style fit. Historic fit B approximates the exchange term by a constant. Historic fit C is derived from the semi-classical arguments, specifically a $Z(Z-1)$ dependence. Historic fit E includes the highest number of terms accounting for the effects of diffuseness, deformation, neutron excess, and similar quantum effects as fit A. Fit E includes some numerical approximations to fit D in Jänecke’s discussion. Fit D has been excluded from this discussion because fits D and E are so similar that they would be indistinguishable on most plots. For the different considerations, the quantity $\Delta E_C$ is determined to be:

$$\Delta E_{CA} = 1.424\bar{Z}A^{-1/3} - 1.237\bar{Z}A^{1/3}[MeV], \quad (5.7)$$
\[ \Delta E_{CB} = 1.430 \bar{Z}A^{-1/3} - .992[MeV], \quad (5.8) \]

\[ \Delta E_{CC} = 1.389Z_\prec A^{-1/3} - 2.041[MeV], \quad (5.9) \]

and

\[ \Delta E_{CE} = 1.539 \bar{Z}A^{-1/3} - 4.470 \bar{Z}A^{-1} \]

\[ +4.4 \bar{Z}A^{-4/3} - .0056 \bar{Z}^2 A^{-2/3} + .06[MeV]. \quad (5.10) \]

The average proton number (\( \bar{Z} \)) is related to the lesser proton number (\( Z_\prec \)) by the following expression:

\[ \bar{Z} = Z_\prec + 1/2. \quad (5.11) \]

A new determination of the Coulomb energy that will be used in this thesis is presented in Section 5.3.1.

5.2.2 Pairing Energy

In this thesis it is demonstrated that the same pairing mechanism that causes the familiar even-even and odd-odd mass staggering, is the origin of the Wigner X term. For this reason, there will be a detailed discussion of the pairing energy.

The pairing term is necessary because like particles pair up to form Cooper pairs, which increases the binding energy. This is taken into account by the final term in the semi empirical mass formula. An odd nucleon cannot pair up, which
will cause a decrease in the total binding energy of a nucleus.

Even-odd mass staggering has long been observed in nuclei. There are formulas that define, $\Delta_n$ and $\Delta_p$, the pairing energies for neutrons and protons, where:

$$\Delta_n(Z, N) = \frac{1}{4} \left( B_E(Z, N-2) - 3B_E(Z, N-1) + 3B_E(Z, N) - B_E(Z, N+1) \right), \quad (5.12)$$

and

$$\Delta_p(N, Z) = \frac{1}{4} \left( B_E(N, Z-2) - 3B_E(N, Z-1) + 3B_E(N, Z) - B_E(N, Z+1) \right). \quad (5.13)$$

These four point formulas are optimal because they best take into account the curvature in the mass parabola caused by the remaining terms in the mass formula. These will result in the global dependence given by the following relation, where the fluctuations have been smoothed out, such that:

$$\bar{\Delta} \approx \frac{12}{A^{1/2}} [MeV]. \quad (5.14)$$

It can be seen in Figures 5.5 and 5.6 that fluctuations in the smooth functional dependence occur which originate from changes in level density. For nuclei with magic numbers, there is a significant gap in the energies at the Fermi surface, and this will result in the pairing gap also increasing. These nuclei are significantly more tightly bound, which is expected when the level density near the Fermi surface is low. Since these fluctuations are a consequence of the shell structure, not of pairing, a similar functional dependence for the BCS pairing gap is used in AutoTAC.
Figure 5.3. The quantity $\Delta_p$ from the four point mass formula, with the general dependence from (5.14). Experimental data from [5]. Magic numbers for the protons are indicated and correspond with peaks.
Figure 5.4. The quantity $\Delta_n$ from the four point mass formula, with the general dependence from (5.14). Experimental data from [5]. Magic numbers for the neutrons are indicated and correspond with peaks.
There are also the simple three point formulas for the pairing gap \( \tilde{\Delta} \), where:

\[
\tilde{\Delta}_n(N, Z) = -\frac{1}{2} \left( B_E(N - 1, Z) - 2B_E(N, Z) + B_E(N + 1, Z) \right),
\]

and

\[
\tilde{\Delta}_p(N, Z) = -\frac{1}{2} \left( B_E(N, Z - 1) - 2B_E(N, Z) + B_E(N, Z + 1) \right).
\]

A three point mass formula was used to calculate the combined quantity \( 2\Delta \), which compares the energy of odd-odd and even-even nuclei [75]. This is defined as:

\[
2\Delta(N, Z) = \frac{1}{2} \left| B_E(N - 1, Z + 1) - 2B_E(N, Z) + B_E(N + 1, Z - 1) \right|.
\]

This is the functional form that will be used in comparisons with the theoretical calculations of Chapter 6. It is the appropriate comparison, because the pairing code was developed and tested for even A nuclei only. The relation has a systematic shift between the energy differences centered about odd-odd and even-even nuclei. The odd-odd nuclei will appear to be lower than the even-even. This results from the residual interaction between the unpaired proton and neutron as well as the curvature caused by the other terms in the mass formula [86], [17].

The combined effects of this residual interaction and the curvature, which
Figure 5.5. Illustration of the $2\Delta$ spacing between even-even and odd-odd mass parabolas. Experimental data from [5].
Figure 5.6. Separation the three point $2\Delta$ formulas for the even-even and odd-odd. Experimental data from [5].
hasn’t been removed gives the following dependence:

\[ 2\Delta_{EE} \approx \frac{34}{A^{1/2}} [MeV], \quad (5.18) \]

and

\[ 2\Delta_{OO} \approx \frac{14}{A^{1/2}} [MeV]. \quad (5.19) \]

The average of these would be expected from (5.14).

5.2.3 Isobaric Mass Multiplet Equation (IMME)

The IMME describes the binding energy of nuclei as a polynomial expansion in the isospin projection [130]. The IMME can be used as a predictive tool for determining the binding energy of unmeasured nuclei [131]. This is written as the following:

\[ B_E(A, T_z) = a(A) + b(A)T_z + c(A)T_z^2. \quad (5.20) \]

This equation can also give insight into a means of calculating the Wigner X from the binding energy after the Coulomb energy is removed from it. In Section 5.3.1 the procedure is described by which the Coulomb energy is removed. This involves a spherical Coulomb fit and the deformation dependent Coulomb correction based on the experimental \( B(E2) \).

Precision measurements, initially for low mass nuclei and modern Penning trap measurements, have verified for mid-mass nuclei, that higher order terms are necessary [117], [95]. This forms the quartic IMME which was originally created to account for second order perturbative corrections to the Coulomb interactions.
The additional terms give the following:

\[ B_E(A, T_z) = a(A) + b(A)T_z + c(A)T_z^2 + d(A)T_z^3 + e(A)T_z^4. \] (5.21)

Removing the Coulomb energy replaces \( B_E \) with \( E_S \) in (5.21), which now has coefficients denoted with a \( (*) \). Figure 5.7 indicates the shell structure effects on the fourth order term.
The Wigner X is given by the following ratio, which is seldom equal to zero:

\[ X(A) \approx \frac{b^*(A)}{c^*(A)}. \]  
(5.22)

5.2.4 Symmetry Energy

The symmetry energy arises from the Pauli exclusion principle and the nucleon-nucleon interaction. It is the primary focus of this investigation. Symmetric nuclear matter, with equal numbers of protons and neutrons, is most stable energetically. The term “nuclear matter” is an idealization that excludes the Coulomb energy. Evaluations of the symmetry energy can be performed along isobaric chains with the Coulomb energy removed. The existence of the linear term in addition to the quadratic dependence in isospin projection \( T_z \) has long been observed \[17\]. This term is called Wigner energy. It is possible to combine the terms in the IMME such that

\[ E_S = b^*|T_z|(|T_z| + X), \]

which defines the quantity \( X \), which will be referred to as the “Wigner X”.

Bohr and Mottelson state that an estimate of \( X = 1 \) reproduces the experimental evidence from nuclei near the \( N = Z \) line on average \[17\]. It has been observed that the value of \( X \) scattered around 1, but in the region with \( A \geq 80 \) the value of \( X \) is 4 \[70\]. Various theoretical arguments are capable of justifying various values of \( X \), but none of them thus far have provided an explanation of the variations in \( X \). In Chapter \[6\] it is demonstrated that strong isovector pairing results in a value of \( X = 1 \). Deviations are caused by variations in level density due to shell structure and attenuation of the pairing correlations. This interpretation intimately relates the Wigner X with even-odd staggering of the binding energies.
5.3 Analysis of Experimental Data

Experimental binding energies exists for \( N = Z \) nuclei up to \( A = 80 \) in the Audi Mass Evaluation \([5]\). Beyond this the experimental measurements are replaced by phenomenological extrapolations up to \( A = 100 \). The extracted experimental values of \( X \) have errors resulting from experimental uncertainties and the Coulomb energy removal.

5.3.1 Coulomb Energy Used

The fit of the Coulomb energy for a spherical nucleus will be discussed first. However, because the Coulomb energy also depends on deformation, additional experimental information, specifically the \( B(E2) \) values, will be used. This will be taken into account later by use of \((5.3.1)\).

A MS style of fit was used to calculate the spherical Coulomb energy\([91]\). This fit is of the form:

\[
E_{CMS} = \frac{3}{5} \frac{q^2}{4\pi \epsilon_0 r_0} Z^2 A^{-1/3} \left( 1 - \frac{5}{6} \left( \frac{d\pi}{r_0} \right)^2 A^{-2/3} - 5 \left( \frac{3}{16\pi} \right)^{2/3} Z^{-2/3} \right). \tag{5.23}
\]

The first correction to the classical expression, \((5.3)\), takes into account nuclear diffuseness. The second is the exchange correction which is necessary because protons obey the Pauli principle and wave-functions cannot completely overlap \([67]\).

The fit includes 2 parameters which are the radius parameter \((r_0)\), and the diffuseness \((d)\) of the nuclear surface.
Figure 5.8. Comparison of various historic fits from Jänecke for the difference in energy for mirror nuclei, which are what is typically used to calibrate. These are color coded by their isospin projection ($\pm T_z$) and come from [5].
Figure 5.9. Linear Coulomb fit, after careful change of variables, used in the analysis of the Wigner X. Experimental data from [5].
Combining (5.23) and (5.6), results in the following expression:

\[
\Delta E_{CMS} = \frac{3}{5} \frac{q^2}{4\pi \epsilon_0 r_0^2} 2 \bar{Z} A^{-1/3} \left( 1 - \frac{5}{6} \left( \frac{d\pi}{r_0} \right)^2 A^{-2/3} - \frac{10}{3} \left( \frac{3}{16\pi} \right)^{2/3} \bar{Z}^{-2/3} \right). \tag{5.24}
\]

For mirror nuclei, the average proton number \( \bar{Z} = \frac{A}{2} \), such that \( \frac{\bar{Z}}{A} \) is a constant equal to \( \frac{1}{2} \). The finite difference approximation is reliable, and a plot of \( \Delta E_{CMS} \) against the quantity \( \bar{Z} A^{-1/3} \) falls along a line as demonstrated in Figure 5.9. For mirror nuclei, this fit is similar to Historic Fits A and B. Only even A nuclei will be used to determine the Wigner X, and for this reason, only even A mirror nuclei were included in this evaluation of the Coulomb energy.

This fit was performed using the experimental binding energies of 73 pairs of mirror nuclei for \( A > 20 \) found in the LBNL Table of Atomic Masses compiled from the Audi Mass Evaluation [5]. From the linear fit, shown in Figure 5.9, the following relation for the Coulomb energy difference of mirror nuclei is found:

\[
\Delta E_{CMS} = 1.461(\pm 0.008) \bar{Z} A^{-1/3} - 1.113(\pm 0.039) [MeV]. \tag{5.25}
\]

The slope of the fitted line gives an radial parameter with \( r_0 = 1.183 \pm 0.006 \text{ fm} \) and the first term in the general equation. According to (5.24), the slope, and offset are related to each other. \( r_0 \) is fixed from the slope and the offset terms are worked out by removing the mirror nuclei restriction that \( \bar{Z}/A = \frac{1}{2} \), for the two corrections. The coefficient for the last correction, the Coulomb exchange correction, was chosen to be \( 5\frac{3^{2/3}}{16^{2/3}/\pi^{2/3}} \), as suggested by (5.23). This allows for the determination of the parameter \( d \), such that:

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\[ \Delta E_{CMS} = 1.461(\pm 0.008) \bar{Z}A^{-1/3} \]

\[-1.045(\pm 0.078) \bar{Z}A^{-1} - 0.744(\pm 0.004)(\bar{Z}/A)^{1/3}[MeV]. \quad (5.26)\]

All of the terms in (5.23) are multiplied by the radius, and therefore radial error will cause an error in all. OriginPro 8 was used to calculate the adjusted \( R^2 \) and reduced \( \chi^2 \), which measure how appropriate a fit is. The resulting values are \( R^2 = 0.99808 \) and \( \chi^2 = 307.034 \).

Integrating the above result, using (5.6), the Coulomb energy is determined to be the following:

\[ E_{CMS} = 0.731(\pm 0.004)Z^2A^{-1/3} \]

\[-0.523(\pm 0.039)Z^2A^{-1} - 1.116(\pm 0.006)Z^{4/3}A^{-1/3}[MeV]. \quad (5.27)\]

Now deformation effects are taken into account, using experimental \( B(E2) \) values. The \( B(E2) \) values are converted into \( \varepsilon_2 \) deformations using (2.17) and (2.20), such that:

\[ E_S = -B_E + 0.731Z^2A^{-1/3} - 0.523Z^2A^{-1} - 1.116Z^{4/3}A^{-1/3} \]

\[ + \frac{3}{5} \frac{e^2Z^2}{4\pi\varepsilon_0r_0} \left( B_c(\varepsilon_2, \gamma) - 1 \right), \quad (5.28)\]
where

\[ B_c(\varepsilon_2, \gamma) \approx 1 - 1.429\varepsilon_2^2 - 0.045\varepsilon_2^3\cos(3\gamma). \] (5.29)

One source of error in \( E_S \) results from the experimental error associated with the \( B(E2) \) values.

There is a secondary source of error coming from the fact that the \( B(E2) \) values give no information about the sign of the deformation, that is, if a nucleus is oblate or prolate. This uncertainty is generally smaller than the experimental \( B(E2) \) error. Additional information coming from the rotational band structure can be used for most nuclei to determine if they are oblate or prolate. However, in the region of interest \( A \approx 80 \) is where the nuclei are transitional, and this is also where the magnitude of this uncertainty is the largest. For this reason, the entire set of data was treated consistently using the average of the combined \( B_c \) of oblate and prolate shapes, with the secondary error coming from half the difference.

5.3.2 Wigner X

After the removal of Coulomb energy, the fourth and third order terms in (5.21) turn out to be small compared to the linear and quadratic terms as shown in Figure 5.7. In addition, the theoretical calculations in Chapter 6 allow only 3 steps in \( T_z \). For these reasons, the quadratic expression for \( E_S(T_z) \) is assumed in the evaluation of the Wigner X. This is done in the same manner for the extraction of X from the experimental and theoretical values of \( E_S \), such that:

\[ E_S = b^*|T_z|(|T_z| + X). \] (5.30)

With this form of the symmetry energy, the X term can easily be solved for.
The first derivative is given by the difference in $E_S$ for two nuclei which have $\Delta T_z = 2$ along an isorotational sequence, with:

$$\frac{\partial E_S}{\partial T_z} \bigg|_{T_z = \bar{T}_z} \approx \frac{\Delta E_S}{\Delta T_z} \bigg|_{T_z = \bar{T}_z} = 2c(\bar{T}_z + X/2).$$  \hfill (5.31)

Considering that (5.31) is a linear function in $\bar{T}_z$, it will have an x-intercept which can be solved for. The Wigner X is related to the x-intercept by a factor of $-2$. 

Figure 5.10. The even-even parabola used in determining the Wigner X. Experimental data from [5].
Figure 5.11. The first derivative of even-even parabola indicating the x-intercept used in determining the Wigner X. Experimental data from [5].
Three point formulas, similar to that used in calculating the pairing gap, have been used on the neutron rich nuclei nearest to the $N = Z$ line. These are defined as:

$$X_E(A) = \left( \frac{6E_S(T_z = 0) - 8E_S(T_z = 2) + 2E_S(T_z = 4)}{-E_S(T_z = 0) + 2E_S(T_z = 2) - E_S(T_z = 4)} \right),$$

and

$$X_O(A) = \left( \frac{8E_S(T_z = 1) - 12E_S(T_z = 3) + 4E_S(T_z = 5)}{-E_S(T_z = 1) + 2E_S(T_z = 3) - E_S(T_z = 5)} \right).$$

The quantity $X_E$ is for the isobaric chain with even $T_z = [0, 2, 4]$ and $X_O$ for odd $T_z = [1, 3, 5]$. These formulas will be used to calculate the theoretical values of the Wigner X, which will be compared with the experimental results in Chapter 6.

Odd-odd Nuclei along the $N = Z$ line with $A > 76$ have been shown to have isospin inverted states where the ground state has $T = 1$ instead of $T = 0$ [52]. The energy difference caused by this is minimal, on the order of a few hundred keV [69]. In the evaluation of the Wigner X, only even-even nuclei were used.

The small error bars for the lower mass region are primarily caused by the error in the spherical Coulomb energy. The large errors of the $74 \leq A \leq 80$ region are caused by the large experimental $B(E2)$ error. The error bars are also considerably larger in the $A > 80$ region, because of the large error in binding energy of the nucleus nearest to or at $N = Z$. These binding energies are actually extrapolated values, denoted by hollow symbols. This was proposed as being a possible cause of the apparent increase in $X$ [70]. It should be noted that the data sets and the removed Coulomb energy are not the same as those used by Jänecke.
Figure 5.12. The experimental Wigner X, derived from (5.32) and (5.33). 33 isobaric chains were evaluated using experimental data from [5]. This will be used to make comparisons with the calculations described in Chapter 6. The indicated errors come from the experimental binding energy error and the error in the Coulomb energy. A transition to larger X is observed near A=80. Also, it should be noted that as A approaches a doubly magic number, the X appears to dip down and then up. The X values from Jänecke et al. have been included from [70].
6.1 Isospin

Isospin was introduced to explain the symmetries between protons and neutrons [59]. Both have nearly identical mass and the same strong interaction with other nucleons.

In second quantization the isospin operators are defined in the following way:

\[
\hat{T}_z = \frac{1}{2} \left( \sum_k \hat{n}_k^+ \hat{n}_k - \sum_k \hat{p}_k^+ \hat{p}_k \right),
\]

(6.1)

\[
\hat{T}_+ = \sum_k \hat{n}_k^+ \hat{p}_k,
\]

(6.2)

and

\[
\hat{T}_- = \sum_k \hat{p}_k^+ \hat{n}_k.
\]

(6.3)

The operators obey the same commutation relations as the angular momentum operators \( L_z \) and \( L_\pm \). In the above expressions, \( \hat{n}_k^+ \) creates a neutron and \( \hat{p}_k^+ \) creates a proton. The neutron and proton carry isospin of \( \frac{1}{2} \) and isospin projection of \( \pm \frac{1}{2} \), respectively.
The two-body Hamiltonian, described in Chapter 2, conserves isospin. This means that the Hamiltonian is invariant under a rotation in isospace, which is an abstract rotation generated by the isospin operators. This is analogous to spatial rotations generated by the operators of orbital angular momentum.

6.1.1 Spontaneous Symmetry Breaking

Isorotational invariance implies that the eigenfunctions of the Hamiltonian have $T$ and $T_z$ as good quantum numbers. In other words, these quantum numbers reflect isospin symmetry conservation. However, if the pairing correlations are calculated by means of the BCS mean field approach, the isorotational invariance is broken. The pair field, used in this approach behaves as a vector under isorotation. The isospin symmetry is spontaneously broken by the mean field, and all orientations of the pair field are equivalent \[45\]. Theoretical calculations, in which the isospin symmetry is restored, will be shown to produce a Wigner X term that is comparable to the experimentally determined values in Chapter 5.

As stated previously, most mean field calculations treat pairing of protons and neutrons separately. For nuclei with significantly different numbers of neutrons and protons, this approximation is valid. However, for nuclei with approximately equal numbers of neutrons and protons, the proton-neutron pair interaction is important. The isovector ($T = 1$) neutron-proton pair correlations must be taken into account in order to restore the isospin symmetry.

Isospin symmetry is approximately restored by the means of the isorotational energy term described below. For strong symmetry breaking by a large isovector pair field, a isorotational band structure emerges for the symmetry energy $E_S$. This is analogous with the energy of a rotational band ($E_L$) of a deformed nucleus.
The rotational band of a well deformed nucleus contains a sequence of states with the following L-dependence \[ E_L = \frac{\hbar^2}{2I} L(L + 1). \] \hspace{1cm} (6.4)

Here, \( L \) is the angular momentum and \( I \), the moment of inertia of the nucleus. The addition of 1 is a quantum mechanical result which reflects the fact that the three components of angular momentum do not commute. The analogous isorotational band should have the same \( T \)-dependence:

\[ E_S \propto T(T + 1). \] \hspace{1cm} (6.5)

In the ground state of even-even nuclei, \( T = |T_z| \).

6.1.2 Wigner X Background

As shown in Figure 5.12, the experimental values of X fluctuate substantially about \( X = 1 \). The low A region appears to contain a rough \( X = 1 \) signature as
was described previously. It will be demonstrated that the deviations from $X = 1$

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6.2 Exact Solution of the Isovector Pairing Problem

There are various approximate approaches that can be applied to the nuclear pairing problems, which are discussed in Appendix A. These all start with the BCS mean field solutions which generates a common problem. The methods become unreliable, near the critical pairing strength, where the BCS pairing gap \( \Delta \to 0 \) [7].

Various new approximate techniques were developed in this thesis in order to address the pairing problem. Each of these were eventually found to be poorly suited for describing the Wigner X. They are described in some detail in Appendix B. Not included is an attempt to create a shifted window that will recenter levels used about the respective Fermi surfaces for protons and neutrons, because it was shown to not preserve isospin. In the early phase of this thesis, a SCRPA hybrid model was developed which is described in Appendix B.1. However, this approach was shown to become inaccurate for larger pairing strengths and was abandoned. Instead the pairing problem is solved exactly via matrix diagonalization within a small space of single particle levels.

6.2.1 Hamiltonian with Isovector Pairing

A pure monopole isovector pairing Hamiltonian is used to describe the effects of pairing on the correlated ground state, with:

\[
H = \sum_{k,\tau} (\epsilon_{k,\tau} - \lambda_\tau) \hat{N}_{k,\tau} - G \sum_{kk',\tau'} \hat{P}_{k,\tau'}^+ \hat{P}_{k',\tau'}.
\]  

(6.6)

Here the label \( \tau' \) indicates that the proton, neutron, and mixed proton-neutron pairs are included. The unprimed label \( \tau \) excludes the mixed pair used on the pro-
ton and neutron number operators \( \hat{N}_{k,\tau} \). Using the common phase convention, the operators are defined \([50]\). This is done, such that:

\[
\hat{P}_{k,-1}^+ = \hat{p}_k^+ \hat{p}_k^- \\
\hat{P}_{k,0}^+ = \frac{1}{\sqrt{2}} \left( \hat{n}_k^+ \hat{p}_k^- + \hat{p}_k^+ \hat{n}_k^- \right) \\
\hat{P}_{k,1}^+ = \hat{n}_k^+ \hat{n}_k^-.
\]

This Hamiltonian is invariant under rotations in isospace; in other words it conserves isospin. The matrix elements of this simple interaction consist of the energy sum of occupied levels and the interaction strength. After diagonalization, the resulting ground state energy will have the exact pairing correlations caused by the isovector pairing interaction.

### 6.2.2 Isovector Pairing Software

The computational complexity is dominated by the building of configurations and by diagonalization.

A ternary configuration counter was designed that involves the two sets of levels for protons and neutrons. It counts from a number corresponding to the ground state to a number that is roughly 9 to the power of the number of levels. Clearly, this will be time consuming for large systems, specifically those with 10 or more levels. Configurations are saved if they can be reached by a series of pair excitations from the uncorrelated ground state, having lowest levels occupied.
A far faster counter was also designed. This first builds the ground state then does first and second order pair excitations about it. Successive excitations are then created based on the previous iteration. All configurations are then scanned through and duplicates are removed. This is far faster for smaller systems in calculations that only include the lowest order excitations.

The software library LAPACK (Linear Algebra PACKage) is used for diagonalization. It was written in Fortran 77 and eventually Fortran 90, and is available through the University of Tennessee [2]. It contains routines that solve moderate sized eigenvalue problems such as diagonalization of the pairing Hamiltonian.

More recently, a library has been developed to solve large scale eigenvalue problems. ARPACK (ARnoldi PACKage) is based on LAPACK and is available through Rice University. It can be used to compute the lowest eigenvalues and corresponding eigenvectors of large, sparse matrices. It uses the iterative Lanczos algorithm and takes into account considerations of the numerical stability of a solution [47]. For these calculations, the sparse pairing matrix is stored dynamically, and the time required for the calculation is substantial.

For intermediate D×D matrices, where D ≲ 4000, there is minimal performance improvement using the ARPACK routines compared to LAPACK. However for matrices that are ten or more times larger ARPACK routines are necessary because of the hardware requirements of LAPACK. Unfortunately, calculations of this size cannot be performed in a timely manner. For this reason, LAPACK was used in the following calculations of systems with at most seven levels half filled. When using isovector pairing, this calculation has dimension D= 4145 compared to D= 20 for a calculation with only one nucleon type. Each diagonalization of this size takes slightly less than one hour.
6.3 Six and Seven Level Calculations

As mentioned previously, the computational complexity grows quickly as the number of levels is increased. For this reason, pair correlations are studied within six and seven levels for which numerical diagonalization could be easily carried out. Using the same equations as for the experimental energies, consisting of combined correlated ground state energies produces theoretical values of $2\Delta$ and Wigner X.

6.3.1 Schematic Wigner X Results

The ground state energies were calculated for systems of 12 nucleons on six levels as a function of the isovector interaction strength ($G$). Different level distributions were investigated in order to study the consequences of level bunching, providing insight on the behavior of X from experimental analysis. The Wigner X is calculated as before, by means of (5.32). The results are shown in Figures 6.2 and 6.3.

It is natural to use MeV as the energy scale for the description of nuclei. The first and last levels are at 1 MeV and 6 MeV, respectively. This is comparable with the typical energy scales of the single particle levels. Figure 6.2 demonstrates the effects on the observed X caused by changes in level density. The same levels are used for all $T_z$, corresponding to a constant deformation along the isobaric chain. The system with even level spacing is intended to simulate well deformed nuclei. The gaps in the spectrum simulate the progressive bunching of levels as a nucleus approaches a spherical shape.

In the six level calculations there are six protons and neutrons for $T_z = 0$. For $T_z = 2$ a pair of protons is replaced by a pair of neutrons, and for $T_z = 4$, an addi-
tional pair is switched from protons to neutrons. This is done in accordance with
the Pauli exclusion principle, so that the proton pair is removed from the highest
occupied level, and the neutron pair added is placed on the lowest unoccupied
level.

In the strong pairing limit the isorotational band structure is restored and
$X = 1$. In the no-pairing limit, where $G = 0$, the filling of the levels along
the isobaric chain will dictate the apparent $X$. (5.32) can be used to calculate the
unpaired values of $X$. For example, in the case of evenly spaced levels, where $\Delta E$ is
the level spacing. Replacing the first pair gives $E_S(T_z = 2) - E_S(T_z = 0) = 2\Delta E$,
and the second pair gives $E_S(T_z = 4) - E_S(T_z = 2) = 6\Delta E$. This will cause the
numerator to be equal to zero, giving $X = 0$. Another example is the case of a
highly degenerate level, indicated by the color gold. There is no difference in the
unpaired energy denominator is zero and therefore the $X$ is undefined. For finite
weak pairing, the solution is $X \approx \lim_{\Delta E \to 0} \frac{\Delta E}{\Delta E} = 1$.

Clearly, the position of the energy gap relative to the $N = Z$ Fermi surface will
dramatically influence the $X$ results. The gap of the levels seen for the isobaric
chains approaching the Fermi surface generate the down-up phenomena for chains
approaching doubly magic nuclei, as seen in Figure 5.12. These fluctuations will be
the largest in the weak pairing limit ($G \to 0$). They are attenuated by increasing
$G$. For realistic values of $G$, this attenuation is substantial, and scattering around
$X = 1$ is expected.

As will be discussed later, there is some indication that the deformation will
generally be decreasing along the isobaric chains in the $A \approx 80$ region. Figure 6.3
is intended to simulate this, where the level distributions represent a more extreme
scenario than is actually expected. In this scenario, the deformation changes from
Figure 6.2. The Wigner X for various level arrangements corresponding to constant deformation along an isobaric chain. The insert illustrates the levels used in the calculations. The yellow shaded region corresponds to the range of pairing strengths used in the comparison with experiment.
Figure 6.3. The Wigner X for a dynamically evolving level arrangement corresponding to a decrease in deformation along an isobaric chain. This is specifically intended to imitate the $A \approx 84$ region.
highly deformed to spherical over the range from $T_z = 0$ to $T_z = 4$. This indicates that the $X$ will increase when the levels change, in this way, as a function of $T_z$.

Overall, in the strong isovector pairing limit the value of $X$ is 1. This is expected for operators in the SU(2) group, such as our pairing operators. For moderate pairing strengths and as a result of varying deformation, the values of $X$ have fluctuations about 1, as seen in experiment. Moreover, large fluctuations around the doubly magic nuclei ($A = 40, 56$ and $100$) are explained with this model as coming from the filling of nuclei in the presence of large gaps in the nuclear levels.

6.3.2 $2\Delta$ Results

The procedure for calculating the realistic results is similar to that of the schematic models. A six or seven Nilsson level window, centered about the Fermi surface, was chosen based on the equilibrium deformation. The ground state energy for $T_z = [0, 2, 4]$ or $T_z = [1, 3, 5]$ was calculated for various pairing strengths. The sum of the energies of all occupied levels that were left out of the small window is also included. This sum plays an important role in allowing calculations of $X$ to be performed along an isobaric chain with changing deformation.

The levels resulting from AutoTAC deformations were used to calculate the Wigner $X$ as well as the pairing gap $2\Delta$. The energy differences along an isobaric chain are used calculate $2\Delta$ as defined in (5.17). This observable has the advantage of not being dependent on the removal of the Coulomb energy. In addition, this observable appears not to be sensitive to the deformations used. The results can also be compared with the phenomenologically observed $A$ dependence described by (5.18).
TABLE 6.1

PAIRING STRENGTHS USED IN THEORETICAL PAIRING CALCULATIONS

<table>
<thead>
<tr>
<th>A</th>
<th>G</th>
</tr>
</thead>
<tbody>
<tr>
<td>36 ≤ A ≤ 46</td>
<td>1.5 MeV</td>
</tr>
<tr>
<td>48 ≤ A ≤ 58</td>
<td>1.4 MeV</td>
</tr>
<tr>
<td>60 ≤ A ≤ 70</td>
<td>1.3 MeV</td>
</tr>
<tr>
<td>72 ≤ A ≤ 82</td>
<td>1.2 MeV</td>
</tr>
<tr>
<td>84 ≤ A ≤ 94</td>
<td>1.1 MeV</td>
</tr>
<tr>
<td>96 ≤ A ≤ 100</td>
<td>1.0 MeV</td>
</tr>
</tbody>
</table>

The pairing strength is shifted linearly from 1.5 MeV for the low mass region to 1 MeV the high mass region. This is shown in Table 6.1. This intermediate pairing strength generates a substantial mixing of many pair excited configurations. The decrease in the pairing strength is closely related to the decrease in the average level spacing as the mass number is increased. The same pairing strength was used for the X calculations.

For the $2\Delta$ calculations, odd-odd nuclei are needed. The deformations for the odd-odd nuclei are taken as being the average of the deformations of the adjacent even-even nuclei, as calculated in AutoTAC. For the adopted values, the deformations of the neighboring nuclei with $T_z - 1$ are used. The results are shown in Figure 6.4. The calculations centered at $T_z = 0$ and $T_z = 1$ indicate that the pairing strength used is realistic and can be used to calculate the X observable in
Figure 6.4. The pairing $2\Delta$ for centered about even-even nuclei. Peaks are seen for doubly magic nuclei. For $T_z = 0$, the experimental values of $2\Delta$ are substantially larger than predicted by the model. Experimental data from [5].
the symmetry energy. An increase of $2\Delta$ that is observed experimentally for the even-even $T_z = 0$ nuclei is not reproduced by these calculations. The structure of the $T = 0$ state in the odd-odd nuclei prevents any enhancement of pairing correlations, which will result in a $2\Delta$ larger than typical [122, 50].

6.3.3 Wigner X Results

The calculation of the Wigner X involves the six and seven Nilsson level systems based on the AutoTAC deformations using the same pairing strength as in the $2\Delta$ calculations. The results are shown in Figure 6.5. As expected from the schematic results, in some of the regions the experimental values are reproduced. In particular, near double magic nuclei, where the deformation is essentially constant and small. In these regions, the calculated X shows the same up and down fluctuations, which are seen experimentally. Clearly, the pairing correlations in nuclei are not strong enough to average out effects from level bunching.

Tables 6.2-6.7 compares the $\varepsilon_2$ deformation parameter from the experimentally measured $B(E2)$ values, the values from the AutoTAC evaluations, and the values from Möller-Nix [96], [81]. Typically, the $B(E2)$ values used in these tables, from Raman et al., are adopted values. Global values are sometimes used and are marked with an (*).

Generally, the X results based on the AutoTAC deformations overestimate the amplitude of the oscillation, particularly in the $A \approx 52$ region. This is the first indication that some incorrect deformations are being used. As shown in Figure 6.2 the amplitude of the fluctuations is typically largest for substantial bunching of levels, with the exception of value of $X = 1$ when the calculation is centered about a highly degenerate level. Tables 6.2 and 6.3 include an experimentally determined
Figure 6.5. The Wigner X from experiment compared with two deformation dependent calculations, the first of which, in red, involves using AutoTAC deformations. The second, in dark blue comes from adopted deformations. Modified experimental data from [5].
value of $\varepsilon_2$, based on the measured $B(E2)$, which appear to be substantial. This disagrees with the calculated spherical deformations used.

The opposite problem occurs for $A \approx 84$. The theoretical fluctuations are small in amplitude when compared to experiment. The AutoTAC deformations are again small, but the experimental evidence, included in Tables 6.5 and 6.6 indicates that the deformations are initially large and get smaller as $T_z$ increases. The experimental deformations imply that the levels evolve in a similar manner as was modeled previously in Figure 6.3. Meanwhile, the corresponding theoretical deformations are small, and the calculations involve highly degenerate levels resulting in $X = 1$.

The model based on AutoTAC deformations and any other model used to calculate $X$, will be limited by the deformations used. A related issue, in the $74 \leq A \leq 88$ region, is caused by a competition between energy minima at oblate, and prolate shapes of moderate deformation and a third substantial deformation at $\varepsilon_2 \approx 0.38$.

Additional information about the deformation is required to improve the calculations of $X$. The rotational band structure of the studied nuclei provides additional insight. As an example of this, the $A = 80$ nuclei used are shown in Figure 6.6 [118]. The experimental rotational frequency $\omega$ is defined by the following relation:

$$\omega(I) = \frac{E(I) - E(I + 2)}{2}.$$  \hfill (6.10)

The linear increase of $I(\omega)$ indicates a good rotor, which has large deformations ($\varepsilon_2 > .2$). The strong upward bending in $^{80}$Kr is characteristic of a transitional nucleus with large shape fluctuations about a small equilibrium deformation ($\varepsilon_2 \lesssim$
2). A vertical line indicates a vibrational nucleus with very small deformation ($\varepsilon_2 \lesssim .1$). Details are described by Frauendorf et al. [44].

Combining the calculated equilibrium deformations with the experimental deformation and the information from the rotational band structure, the set of adopted deformations was constructed. Generally, the small theoretical deformations were assigned a value $\varepsilon_2 \lesssim .15$, in order to account for shape fluctuations. The effective deformation of the ground state should be smaller than the experimental value derived from the $B(E2; 2^+_1 \rightarrow 0^+_1)$, because the latter represents an average of the deformations corresponding to the $0^+$ and $2^+$ levels.

In many cases where there was some uncertainty in the choice of adopted deformations, this freedom was used to slightly adjust the deformation such that the experimental values of X are reproduced. The adopted values are also included in Tables 6.2-6.7. The resulting X is included in Figure 6.5. Impressive agreement, with the experimentally determined X, can be achieved.
Figure 6.6. The rotational band structure for $A = 80$ nuclei of interest for the Wigner X evaluation. Here, a line with an initial backward slope indicates a spherical nucleus, a nearly vertical saw-tooth shape indicates $\varepsilon_2 \approx = \pm 1$, and flat lines with positive slope indicate larger deformations.
### TABLE 6.2

**QUADRUPOLE DEFORMATION PARAMETER $\varepsilon_2$ FOR**

$36 \leq A \leq 46.$

<table>
<thead>
<tr>
<th>$A$</th>
<th>$Z$</th>
<th>Nilsson</th>
<th>Wood-Saxon</th>
<th>Möller-Nix</th>
<th>Experiment</th>
<th>Adopted</th>
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<td>±0.232</td>
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TABLE 6.3

QUADRUPOLE DEFORMATION PARAMETER $\varepsilon_2$ FOR $48 \leq A \leq 58$.

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<th>Z</th>
<th>Nilsson</th>
<th>Wood-Saxon</th>
<th>Möller-Nix</th>
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<td>Wood-Saxon</td>
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<td>0.375</td>
<td>±0.356*</td>
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<tr>
<td>78</td>
<td>34</td>
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<td>78</td>
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<td>±0.249</td>
<td>-0.200</td>
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<tr>
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<tr>
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<tr>
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<td>0.050</td>
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<td>-0.300</td>
</tr>
<tr>
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TABLE 6.6

QUADRUPOLE DEFORMATION PARAMETER $\varepsilon_2$ FOR

$84 \leq A \leq 94$.

<table>
<thead>
<tr>
<th>A</th>
<th>Z</th>
<th>Nilsson</th>
<th>Wood-Saxon</th>
<th>Möller-Nix</th>
<th>Experiment</th>
<th>Adopted</th>
</tr>
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<tr>
<td>84</td>
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<td>0.000</td>
<td>0.000</td>
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<td>±0.202</td>
<td>0.150</td>
</tr>
<tr>
<td>84</td>
<td>40</td>
<td>0.000</td>
<td>0.000</td>
<td>0.050</td>
<td>±0.236</td>
<td>0.200</td>
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<td>0.050</td>
</tr>
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<td>0.000</td>
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<tr>
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<td>0.000</td>
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<tr>
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<td>0.050</td>
<td>±0.183*</td>
<td>0.150</td>
</tr>
<tr>
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<td>±0.158*</td>
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</tr>
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<td>±0.180*</td>
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</tr>
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<td>±0.099</td>
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<tr>
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<td>±0.162*</td>
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<td>0.050</td>
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<td>±0.142</td>
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</tr>
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</table>
## Table 6.7

**Quadrupole deformation parameter $\varepsilon_2$ for $96 \leq A \leq 100$.**

<table>
<thead>
<tr>
<th>A</th>
<th>Z</th>
<th>Nilsson</th>
<th>Wood-Saxon</th>
<th>Möller-Nix</th>
<th>Experiment</th>
<th>Adopted</th>
</tr>
</thead>
<tbody>
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<td>±0.148</td>
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<td>0.025</td>
<td>±0.121</td>
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</tr>
<tr>
<td>96</td>
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<td>0.000</td>
<td>0.000</td>
<td>0.042</td>
<td></td>
<td>0.050</td>
</tr>
<tr>
<td>98</td>
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<td>0.000</td>
<td>0.108</td>
<td>±0.183</td>
<td>0.100</td>
</tr>
<tr>
<td>98</td>
<td>46</td>
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<td>0.000</td>
<td>0.042</td>
<td>±0.153</td>
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</tr>
<tr>
<td>98</td>
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<td>±0.120</td>
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CHAPTER 7

SUMMARY AND RESULTS

The AutoTAC computer code was constructed to generate Potential Energy Surfaces (PES) by means of the Strutinsky micro-macro method using both deformed Wood-Saxon (WS) and Nilsson (MHO) levels. The PES contain minima determining the equilibrium deformation parameters, such as $\varepsilon_2$, which are similar to the commonly used results by Möller and Nix. Preference for the use of one compared with the other, based on the experimentally determined deformations, varies from case to case.

The PES were then used as a starting point for calculations of the electromagnetic dipole strength function, the low energy spectrum, and the linear symmetry energy term of nuclei of astrophysical relevance. More accurate calculations of binding energies of $N \approx Z$ nuclei should include the Wigner X term calculated from a microscopic foundation. A microscopic calculation of the absorption probability of dipole radiation can be performed using the Instantaneous Shape Sampling (ISS) method.

Both of these problems have an astrophysical motivation, because they improve the nuclear input necessary for various scenarios of astrophysical processes which are mediated by nuclear reactions. Additionally, they address problems which are interesting from a nuclear structure perspective.
The motion of the nuclear shape fluctuations is about ten times slower than the oscillations of the neutrons against the protons or GDR. Based on this observation, the ISS method for calculating the photo-absorption cross-section in the astrophysically relevant energy region is suggested. It was applied to transitional nuclei which have fluctuating deformations. This was done by combining ground state probability distributions with the dipole strength function for each shape present, calculated by means of the QRPA. The total strength function is taken as the sum of all individual strength functions, weighted with their respective probabilities.

There were three approaches used to generate the probability distributions. The first used axial TAC potential energies and a simple kinetic energy term with a constant mass parameter. The erratic dependence on a the mass parameter clearly limited the predictive potential of this approach. A second approach involved a deformation based configuration hopping picture similar to that which is used to describe pairing on a lattice. Unfortunately, the resulting $B(E2)$ transition strengths were too small, while the excited $E(0^+)$ states were too large.

The third approach is based on the Interacting Boson Model (IBM). The IBM is known to account well for the lowest collective quadrupole excitations of both well deformed and transitional nuclei. The IBM parameters $\zeta$, $\chi$, and $e_B$ were determined, using three energy ratios and a $B(E2)$ transition probability ratio. From this, the IBM Hamiltonian generated a set of localized states onto which the ground state was projected, giving the probability of the instantaneous shape.

The entire ISS procedure was applied to nuclei for which experimental cross-sections, in the astrophysically relevant low energy region, have recently been measured. It provides an accurate description of the photo-absorption cross-section
in the low energy region.

It seems promising to combine the IBM mapping technique with the ISS. The mapping technique can predict the IBM parameters for exotic nuclei far from stability. This can be used to calculate cross-sections of nuclei of interest in the r-process.

A new IBM mapping technique was developed in this thesis, which projects the fermionic AutoTAC PES onto a bosonic IBM PES. The AutoTAC potentials have a one to one correspondence with potentials generated in the IBM. This allows for the use of a root mean squared minimization procedure to solve for the three unknown IBM parameters $\zeta$, $\chi$, and $c_{\beta}$. The total energy scale $c_E$ is defined by calculating the $E(2^+_1)$ in TAC. Surprisingly good results are found using the simplest IBM-1 Hamiltonian with a constant 10 bosons. The model as presented in this thesis is excellent at producing the low lying energy spectrum and the relevant transition probabilities for slightly deformed nuclei, such as $^{108-116}$Cd and $^{102-112}$Pd. The techniques suggested by Nomura et al. give comparable results. For well deformed nuclei the AutoTAC PES appear to have substantial changes of the curvature. Because of this, a more advanced Hamiltonian is required to properly map these potentials.

The origin of the term proportional to $|N - Z|$ in the nuclear binding energy, also called the Wigner X, has been a topic of interest for years. In this thesis, one previously suggested mechanism, the spontaneous breaking of isorotational symmetry by the isovector pair field, has been shown to generate the term. This will generate a $T(T + 1)$ dependence in the strong pairing limit.

An analysis of the experimental binding energies was done in order to isolate the spherical Coulomb energy using mirror nuclei, which was combined with an ex-
perimentally determined deformation contribution and removed from the binding energy.

This leaves just the strong part of the interaction, which conserves isospin. From these energies the experimental $X$ was determined. The values typically deviate from $X = 1$, as was noticed previously. After closely examining the results, shell structure of the nucleus appears to play an important role.

To verify this observation, a microscopic description of isovector pairing was developed, which goes beyond the common BCS mean-field approximation. The first attempt to solve this problem involved developing a new approach, called the hybrid approach. In this method, a few single particle levels near the Fermi surface are coupled to collective RPA phonons. SCRPA phonons were used to improve results near the critical pairing strength, with limited success because the accuracy of the model was not as good as expected.

A more simple technique was used which involved direct diagonalization of the pairing Hamiltonian for small few level systems. Time and hardware constraints limited these calculations to contain seven levels at most. Preliminary calculations with model levels provide great insight into some of the observed experimental fluctuations.

Calculations using realistic single particle levels resulting from the MHO produce an $X$ comparable with the experimental $X$. This justified the assertion that the single particle level density was important in causing the fluctuations. A related quantity, the nuclear deformations was found to cause the remaining discrepancies.

Theoretical calculations of the equilibrium deformation using the MHO, WS potential, and folded Yukawa potential do not always agree with the experimen-
tally determined deformation. This ambiguity was resolved using the theoretically calculated deformations in addition to the experimentally measured $B(E2)$ values and rotational band energies. The resulting set of adopted deformations is able to reproduce the $X$ fluctuations for all $A$ used, which demonstrates that, the Wigner $X$ term can be calculated in a microscopic way using an isovector pairing interaction.

The consequences of a spin zero isoscalar-isovector pairing interaction was briefly studied. For this type of interaction, $X = 2$ was found in the limit of strong and equal isovector and isoscalar pairing strength. There is considerable uncertainty in the isoscalar strength and because of the success of the before mentioned pure isovector pairing scenario, this model was not fully tested. The good agreement of the Wigner $X$ calculated from a pure isovector pair interaction seems to indicate that the isoscalar correlations are relatively weak.

Various truncations techniques of the full configuration space were developed, allowing for up to 10 levels to be included in the isovector pairing calculations. One particularly promising truncation technique involves calculating the isospin projected BCS wave function which can be used to determine which configurations will have the strongest correlations with the ground state.

An isospin projected BCS model may prove to be the most applicable way of conserving isospin in microscopic calculations. Also, an isovector version of the SCQRPA with LN particle number projection may produce the desired result.

Overall, improved understanding of the mechanisms that cause fluctuations in the Wigner $X$ has been achieved. In addition, the combination of various techniques described in this thesis, now allows for predictive calculations of the photo-absorption cross-section of transitional nuclei far from stability.
APPENDIX A

APPROXIMATE PAIRING APPROACHES

Approximate methods are necessary for describing pairing in large systems. Exact calculations have been performed for, on the order of, 24 half filled levels. This is the case when using one type of identical nucleons. For the case of isovector pairing there are 2 types of nucleons, which greatly increases the dimension of the problem.

For very large systems, approximations such as those based on the BCS and the RPA are commonly used. Both have shortcomings, but they will be discussed because they can provide great insight into pairing problem. For simplicity, the discussion of approximate pairing techniques will be restricted to identical nucleon pairing. The same methods are used in solid state physics for the description of superconductivity.

A.1 BCS Pairing

The simplest approximation for the monopole pairing Hamiltonian assumes constant interaction strength $G$, such that:

$$H = \sum_k (\epsilon_k - \lambda) \hat{N}_k - G \sum_{kk'} \hat{P}_k^+ \hat{P}_{k'}.$$
The pair creation operator \( \hat{P}_k^+ \) creates two particles on a given level in the
the time reversed states \( k \) and \( \bar{k} \). It is written as:

\[
\hat{P}_k^+ = \hat{a}_k^+ \hat{a}_{\bar{k}}^+.
\]

Similarly, the pair removal operator will remove a pair. The number operator
\( \hat{N}_k \) is defined in the following way:

\[
\hat{N}_k = \hat{a}_k^+ \hat{a}_k + \hat{a}_{\bar{k}}^+ \hat{a}_{\bar{k}}.
\]

The BCS wave-function, originally designed to describe the ground state of a
superconductor, was quickly applied to nuclei [19]. Surprisingly, it does a good
job of representing the ground state wave-function of an even-even nucleus [98].
The BCS wave-function is not an eigenstate of the particle number operator, as
seen by its explicit form:

\[
|BCS⟩ = \prod_k (u_k + v_k \hat{a}_k^+ \hat{a}_{\bar{k}}^+) |0⟩.
\]

Here the subscript \( k \) describes a product that runs over all of the levels. The
coefficients \( v_k \) and \( u_k \) come about from the quasi-particle transformation described
in Chapter 2 and can be written in as functions of two parameters, \( \lambda \) and \( \Delta \), such
that:

\[
v_k^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}} \right).
\]

The BCS coefficients are normalized satisfying the following expression:

\[
u_i^2 + v_i^2 = 1,
\]
Figure A.1. The occupation probabilities of particles ($v_k$) and holes ($u_k$). This indicates that the most important levels are those nearest the Fermi surface. With $\Delta = 0$ the Fermi surface is sharp. Typically, nuclear pairing occurs between the curves described by $\Delta = 1$ and $\Delta = 3$. In particular, calculations should contain 10 to 40 levels.
and

\[ u_k^2 = \frac{1}{2} \left( 1 + \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}} \right). \]

The particle occupation probability is defined in such a way that it is equal to the total number of particles \((\mathcal{N})\), with:

\[ \mathcal{N} = 2 \sum_k v_k^2. \]

This provides the condition that determines the chemical potential \((\lambda)\).

The pairing gap \((\Delta)\) gives an indication of how many levels are correlated. It is determined by the following self-consistency condition:

\[ \Delta = G \sum_k u_k v_k. \]

This is more commonly expressed with the substitution of \(u_k\) and \(v_k\), such that:

\[ \Delta = \frac{G}{2} \sum_k \frac{\Delta}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}. \]

Obviously, this equation has a trivial solution for the uncorrelated case of \(\Delta = 0\). There is a second solution with \(\Delta > 0\) for the correlated case when the pairing strength is above some critical value \((G > G_{\text{crit}})\), where pairs are scattered above and below the Fermi surface.

The equations are non-linear and must be solved using an iterative procedure. A description of Newton’s method for the solution is included in Appendix E.1

The BCS equations can also be solved for a system with an odd particle. The odd nucleon will block the level it occupies \((k_b)\), in order to obey the Pauli
Figure A.2. The BCS pairing gap $\Delta$ as a function of the pairing strength. At $G \approx .17$ the $\Delta$ ceases to be the zero solution. The quasi-particle pairing regime correlated states involve strengths larger than this critical pairing strength ($G_{\text{crit}}$).
exclusion principle, which forbids more than one identical particle from occupying the same state. The odd nucleon BCS equations for this case are as follows:

\[ \mathcal{N} = 1 + 2 \sum_{k \neq k_0} v_k^2, \]

and

\[ \Delta = \frac{G^2}{2} \sum_{k \neq k_0} \frac{\Delta}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}. \]

The energy of the correlated ground state is of particular interest in this thesis, is defined as:

\[ \langle \text{BCS} | H | \text{BCS} \rangle = -\frac{\Delta^2}{G} + 2 \sum_k \left( (\epsilon_k - \lambda + \frac{G^2}{2} v_k^2) v_k^2 \right). \]

For intermediate pairing strengths, the BCS approximation is fairly accurate, but in the weak pairing limit with \( G < G_{\text{crit}} \), only the uncorrelated solution exists. Moreover, the correlated ground state calculated with the BCS formalism will always overestimate the energy. Comparisons with the exact solutions of small systems indicate that this is generally on the order of a few MeV. Unfortunately this is the scale of the energy differences that are used in calculating the Wigner X.

A.2 Pairing RPA Based on the Uncorrelated Ground State

The RPA is based on the quasi-boson approximation treating pairs of fermions as bosons, which leads to violations of the Pauli exclusion principle [55]. In second quantized form, the validity of this approximation can be seen when comparing the commutation relations for a pair of fermions with that of bosons. The additional
terms from the fermionic relation are assumed to be of low amplitude and have random phases, so that essentially, they cancel.

The RPA is used to calculate excited states about a Hartree-Fock vacuum \(|HF\rangle\) [102]. The RPA introduces pair addition (\(A^+_\mu\)) and removal (\(R^+\lambda\)) operators to create the ground states and excited states of the systems with two more and two fewer particles [98]. These are defined as:

\[
\hat{A}^+_\mu |A, 0\rangle = \left( \sum_m X^\mu_m \hat{P}^+_m - \sum_i Y^\mu_i \hat{P}^+_i \right) |A, 0\rangle = |A + 2, \mu\rangle,
\]

and

\[
\langle A, 0 | \hat{R}^+_\lambda = \langle A, 0 | \left( \sum_i X^\lambda_i \hat{P}_i - \sum_m Y^\lambda_m \hat{P}_m \right) = \langle A - 2, \lambda |.
\]

The states contain the so called forward and backward amplitudes, \(X^\mu_k\) and \(Y^\mu_k\), respectively. The square of each indicates the probability of finding the initial states with which they are associated in some excited state \(|\mu\rangle\) or \(|\lambda\rangle\) [98]. Here, subscripts are chosen such that \(k = m\) for unoccupied and \(k = i\) for occupied. The addition and removal operators satisfy the bosonic commutation relations:

\[
\langle A, 0 | [A_\mu, A^+_\mu'] | A, 0 \rangle = \delta_{\mu\mu'},
\]

and

\[
\langle A, 0 | [R_\lambda, R^+_\lambda'] | A, 0 \rangle = \delta_{\lambda\lambda'}.
\]

It is useful to invert the expression for the addition and removal operators, such that:
\[ \hat{P}_m^+ = \left( \sum_{\mu} X_{m\mu} \hat{A}_{\mu}^+ + \sum_{\lambda} Y_{m\lambda} \hat{R}_{\lambda} \right), \]

and

\[ \hat{P}_i^+ = \left( \sum_{\lambda} X_{i\lambda} \hat{R}_{\lambda}^+ + \sum_{\mu} Y_{i\mu} \hat{A}_{\mu}^+ \right). \]

The RPA solution can be expressed in matrix form by combining the equations of motion, coming from the commutation relations of the pair operators with the pairing Hamiltonian. For the addition mode, this is written in the following way:

\[ [H, \hat{A}_{\mu}^+] = \hbar \Omega_{\mu} \hat{A}_{\mu}^+. \]

The full expression is the following:

\[ \begin{pmatrix} A & B \\ -B & C \end{pmatrix} \begin{pmatrix} X_{\mu} \\ Y_{\mu} \end{pmatrix} = \hbar \Omega_{\mu} \begin{pmatrix} X_{\mu} \\ Y_{\mu} \end{pmatrix}. \]

The sub-matrices are defined by the simple expressions:

\[ A_{mm'} = \langle HF \vert [\hat{P}_m, [H, \hat{P}_{m'}^+]] \vert HF \rangle = 2(\epsilon_m - \lambda) \delta_{mm'} - G, \]

\[ B_{mi} = -\langle HF \vert [\hat{P}_m, [H, \hat{P}_{i'}^+]] \vert HF \rangle = -G, \]

and

\[ C_{ii'} = \langle HF \vert [\hat{P}_i, [H, \hat{P}_{i'}^+]] \vert HF \rangle = -2(\epsilon_i - \lambda) \delta_{ii'} + G. \]

The eigenvalues correspond to the excitation energies, such that \( \hbar \Omega_{\lambda} = E_0(A) - \)]
$E_\lambda(A-2)$ and $\hbar\Omega_\mu = E_\mu(A+2) - E_0(A)$. This eigenvalue problem can easily be solved by matrix diagonalization. The dimension is the number of levels, which for nuclear systems are typically relatively small: $N \approx 100$. The forward and backward amplitudes, which result from the diagonalization, are orthogonal and must be normalized so that the following relations are true:

$$\sum_m X_\mu^m X_{\mu'}^m - \sum_i Y_\mu^i Y_{\mu'}^i = \delta_{\mu\mu'},$$

$$\sum_i X_\lambda^i X_{\lambda'}^i - \sum_m Y_\lambda^m Y_{\lambda'}^m = \delta_{\lambda\lambda'},$$

and

$$\sum_m X_\mu^m Y_\lambda^m - \sum_i X_\mu^i Y_{\lambda}^i = 0.$$

The closure relations also apply, such that:

$$\sum_\mu X_\mu^m X_{\mu'}^m - \sum_\lambda Y_\lambda^\mu Y_{\lambda'}^\mu = \delta_{m \mu'},$$

$$\sum_\lambda X_\lambda^i X_{\lambda'}^i - \sum_\mu Y_\mu^i Y_{\mu'}^i = \delta_{i \mu'},$$

and

$$\sum_\lambda X_\lambda^m Y_\mu^m - \sum_\mu X_\mu^m Y_{\mu}^i = 0.$$

Resulting from all of this is a simple expression for the ground state correlation energy, written as:
\[ E_{RPA}^{GSC} = -\sum_{\mu} E_{\mu} \sum_{m} |Y_{m\mu}|^2. \]

This approach gives good agreement between the ground state correlation energies when compared with the exact solution for pairing strength that is well below the BCS critical value. At the critical pairing strength, the lowest solution has \( \hbar \Omega_{\mu} = 0 \).

This, of course, is problematic because it means that there is no energy gained by the addition or removal of pairs. The RPA formalism can also be derived based on the correlated BCS ground state using quasi-particle pairing, which is called pairing QRPA [88]. However, the breakdown at the critical point persists and additional corrections need to be taken into account as illustrated in Figure A.3.

A.3 Renormalized RPA (RRPA) and Self Consistent RPA (SCRPA)

The exact relations, \( \langle HF | \hat{N}_m | HF \rangle = 0 \) and \( \langle HF | \hat{N}_i | HF \rangle = 2 \) are violated for the RPA ground state. The RRPA was developed in order to mend this problem. The RRPA is based on an iterative procedure using renormalized addition and removal operators, which will provide solutions with proper particle number expectation values [28]. These depend on the particle number expectation value \( \langle \hat{N} \rangle \), such that:

\[
\hat{A}_\mu^+ = \left( \sum_m \frac{X_{m\mu}}{\sqrt{1 - \langle \hat{N}_m \rangle}} \hat{P}_m^+ - \sum_i \frac{Y_{i\mu}}{\sqrt{\langle \hat{N}_i \rangle - 1}} \hat{P}_i^+ \right),
\]

and
\[
\hat{R}_\lambda^+ = \left( \sum_i \frac{X_i^\lambda}{\sqrt{\langle \hat{N}_i \rangle - 1}} \hat{P}_i^* - \sum_m \frac{Y_m^\lambda}{\sqrt{1 - \langle \hat{N}_m \rangle}} \hat{P}_m^* \right).
\]

The renormalized pair operators (\( \hat{P}_i^* \)) become the following:

\[
\hat{P}_m^+ = \sqrt{1 - \langle N_m \rangle} \left( \sum_\mu X_m^\mu \hat{A}_\mu^+ + \sum_\lambda Y_m^\lambda \hat{R}_\lambda \right),
\]

and

\[
\hat{P}_i^+ = \sqrt{\langle N_i \rangle - 1} \left( \sum_\lambda X_i^\lambda \hat{R}_\lambda^+ + \sum_\mu Y_i^\mu \hat{A}_\mu^+ \right).
\]

The SCRPA involves the addition of screening factors (\( \langle \hat{P}_i^+ \hat{P}_i^* \rangle \)) to the RRPA. The normalization, orthogonality, and closure relations all remain unchanged from the original RPA. The screening factors result from combined expectation values of the renormalized pair operators:

\[
\langle \hat{P}_m^+ \hat{P}_m^* \rangle = \sqrt{(1 - \langle N_m \rangle)(1 - \langle \hat{N}_m \rangle)} \sum_\lambda Y_m^\lambda Y_m^\lambda,
\]

\[
\langle \hat{P}_i^+ \hat{P}_i^* \rangle = \sqrt{(1 - \langle N_i \rangle)(\langle \hat{N}_i \rangle - 1)} \sum_\lambda Y_i^\lambda X_i^\lambda,
\]

\[
\langle \hat{P}_i^+ \hat{P}_m^* \rangle = \sqrt{\langle \hat{N}_i \rangle - 1(1 - \langle \hat{N}_m \rangle)} \sum_\lambda X_i^\lambda Y_m^\lambda,
\]

and

\[
\langle \hat{P}_i^+ \hat{P}_i' \rangle = \sqrt{\langle \hat{N}_i \rangle - 1(\langle \hat{N}_i' \rangle - 1)} \sum_\lambda X_i^\lambda X_i^\lambda'.
\]

There is some question as to the validity of including a self screening factor which is not removed in the following discussion. The SCRPA can also be
expressed in the form of a matrix eigenvalue problem, with:

\[
\begin{pmatrix}
A^* & B^* \\
-B^* & C^*
\end{pmatrix}
\begin{pmatrix}
X^\mu \\
Y^\mu
\end{pmatrix}
= \hbar \Omega_\mu
\begin{pmatrix}
X^\mu \\
Y^\mu
\end{pmatrix}.
\]

The sub-matrices are defined as:

\[
A^*_{mm'} = 2(\epsilon_m - \lambda)\delta_{mm'} + 2G\sum_{m'}\langle \hat{P}_{m'}^+ \hat{P}^*_m \rangle + \sum_i \langle \hat{P}_{i}^+ \hat{P}^*_m \rangle \delta_{mm'}
- G\frac{\langle 1 - \hat{N}_m - \hat{N}_{m'} + 2\hat{N}_m\hat{N}'_{m'} \rangle}{\sqrt{(1 - \langle \hat{N}_m \rangle)(1 - \langle \hat{N}_{m'} \rangle)}},
\]

\[
B^*_{mi} = -G\frac{\langle 1 - \hat{N}_m - \hat{N}_i + 2\hat{N}_m\hat{N}_i \rangle}{\sqrt{(\langle \hat{N}_i \rangle - 1)(\langle 1 - \hat{N}_m \rangle)}}
\]

and

\[
C^*_{ii'} = -2(\epsilon_i - \lambda)\delta_{ii'} - 2G\sum_{i'}\langle \hat{P}_{i'}^+ \hat{P}^*_i \rangle + \sum_m \langle \hat{P}_{i}^+ \hat{P}^*_m \rangle \delta_{ii'}
+ G\frac{\langle 1 - \hat{N}_i - \hat{N}_{i'} + 2\hat{N}_i\hat{N}'_{i'} \rangle}{\sqrt{(\langle \hat{N}_i \rangle - 1)(\langle \hat{N}_{i'} \rangle - 1)}}.
\]

The following approximation used for simplification:

\[
\langle \hat{N}_m\hat{N}_{m'} \rangle \approx \langle \hat{N}_m \rangle \langle \hat{N}_{m'} \rangle.
\]

In Tables A.1 and A.2 this simplification will be used, labeled (SCRPA), and compared to the result when the problem is solved without use of the approximation, labeled as (SCRPA'). In general, the approximation is quite good, with
discrepancies on the order of a few percent.

Again, the eigenvalue problem is solved via matrix diagonalization. The occupation numbers are defined as functions of the backwards amplitudes, which for weak pairing are small, such that:

\[
\langle \hat{N}_m \rangle = 1 - \left(1 + 2 \sum_{\mu} (Y_{m}^{\mu})^2 \right)^{-1},
\]

and

\[
\langle \hat{N}_i \rangle = 1 - \left(1 + 2 \sum_{\mu} (Y_{i}^{\mu})^2 \right)^{-1}.
\]

The ground state correlation energy for the SCRPA is of the more complicated form \([60]\). This is written as:

\[
E_{SCRPA}^{GSC} = (\epsilon_m - \lambda)\langle \hat{N}_m \rangle + (\epsilon_i - \lambda)\langle \hat{N}_i \rangle - G\langle \hat{P}_{m}^{+} \hat{P}_{m'}^{*} \rangle + G\langle \hat{P}_{m}^{+} \hat{P}_{m'}^{*} \hat{P}_{i}^{*} \rangle + G\langle \hat{P}_{i}^{+} \hat{P}_{m}^{*} \rangle - G\langle \hat{P}_{i}^{+} \hat{P}_{i'}^{*} \rangle.
\]

The SCRPA provides substantial improvement of the ground state correlation energies when compared with the exact solution. The divergence of solutions as they approach the critical pairing strength are almost entirely eliminated, and solutions can be extended slightly past the critical point.
Figure A.3. X calculations compare the isovector QRPA with the exact solution for a 6 level system and a 16 levels QRPA solution with adjusted pairing strength based on $^{100}\text{Sn}$. The isovector calculation was performed using a pairing code from Neergard [88]. Behavior of the QRPA solutions near the BCS critical point appears to be in the region of interest, i.e. in the window where the experimental X is.
TABLE A.1

THE GROUND STATE CORRELATION ENERGIES FOR A SYSTEM WITH 10 EVENLY SPACED LEVELS FOR VARIOUS MODELS [60].

<table>
<thead>
<tr>
<th>G</th>
<th>Exact</th>
<th>RPA</th>
<th>SCRPA</th>
<th>SCRPA'</th>
</tr>
</thead>
<tbody>
<tr>
<td>.00</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>.05</td>
<td>-0.0086</td>
<td>-0.0086</td>
<td>-0.0086</td>
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</tr>
<tr>
<td>.10</td>
<td>-0.0364</td>
<td>-0.0367</td>
<td>-0.0365</td>
<td>-0.0365</td>
</tr>
<tr>
<td>.20</td>
<td>-0.1669</td>
<td>-0.1756</td>
<td>-0.1686</td>
<td>-0.1691</td>
</tr>
<tr>
<td>.30</td>
<td>-0.4350</td>
<td>-0.5419</td>
<td>-0.4424</td>
<td>-0.4497</td>
</tr>
<tr>
<td>.33</td>
<td>-0.5505</td>
<td>-0.8181</td>
<td>-0.5594</td>
<td>-0.5725</td>
</tr>
<tr>
<td>.34</td>
<td>-0.5931</td>
<td>(crit)</td>
<td>-0.6023</td>
<td>-0.6180</td>
</tr>
<tr>
<td>.35</td>
<td>-0.6379</td>
<td>(crit)</td>
<td>-0.6473</td>
<td>-0.6658</td>
</tr>
<tr>
<td>.36</td>
<td>-0.6850</td>
<td>(crit)</td>
<td>-0.6943</td>
<td>-0.7160</td>
</tr>
</tbody>
</table>
TABLE A.2

THE EXCITATION ENERGY OF THE FIRST ADDITION MODE
FOR A SYSTEM WITH 10 EVENLY SPACED LEVELS FOR
VARIOUS MODELS [60].

<table>
<thead>
<tr>
<th>G</th>
<th>Exact</th>
<th>RPA</th>
<th>SCRPA</th>
<th>SCRPA'</th>
</tr>
</thead>
<tbody>
<tr>
<td>.00</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>.05</td>
<td>1.0003</td>
<td>0.9940</td>
<td>1.0005</td>
<td>1.0003</td>
</tr>
<tr>
<td>.10</td>
<td>1.0011</td>
<td>0.9732</td>
<td>1.0034</td>
<td>1.0014</td>
</tr>
<tr>
<td>.20</td>
<td>1.0053</td>
<td>0.8604</td>
<td>1.0279</td>
<td>1.0119</td>
</tr>
<tr>
<td>.30</td>
<td>1.0143</td>
<td>0.5257</td>
<td>1.0970</td>
<td>1.0539</td>
</tr>
<tr>
<td>.33</td>
<td>1.0184</td>
<td>0.2574</td>
<td>1.1266</td>
<td>1.0758</td>
</tr>
<tr>
<td>.34</td>
<td>1.0199</td>
<td>0.2574</td>
<td>1.1266</td>
<td>1.0758</td>
</tr>
<tr>
<td>.35</td>
<td>1.0216</td>
<td>(crit)</td>
<td>1.1481</td>
<td>1.0927</td>
</tr>
<tr>
<td>.36</td>
<td>1.0233</td>
<td>(crit)</td>
<td>1.1592</td>
<td>1.1018</td>
</tr>
</tbody>
</table>
A.4 Self Consistent Quasi-particle Random Phase Approximation (SCQRPA) with Lipkin-Nogami (LN) Particle Number Projection

The SCRPA can be calculated within the quasi-particle formalism. Once again particle number fluctuations will be a setback. It was not long after quasi-particle transformation became a useful tool that the possibility of removing these fluctuations from the wave-functions without losing the essence of the theory, was realized [92]. Lipkin proposed that a modified Hamiltonian could be used to eliminate these effects from the eigenvalues [74]. The LN Hamiltonian contains a correction coming from a power series expansion of the particle number:

\[ H_{LN} = H - N^2 \lambda. \]

This formalism uses a secondary chemical potential. The wave functions generated by this are the same as in the standard BCS, but with a larger \( \Delta \), which remains finite for \( G < G_{crit} \) [93]. The LN method, which makes it possible to more accurately take into account particle number conservation, can be used in the extended scheme of the random phase approximation, resulting in the improved calculation of ground state correlations [89].

The modified BCS coefficients \( \tilde{v}_k \) and \( \tilde{u}_k \) are now defined slightly differently, with:

\[ \tilde{v}_k^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_k - \lambda + 2 \lambda_2 (\tilde{N} + 1)}{\sqrt{(\epsilon_k - \lambda + 2 \lambda_2 (\tilde{N} + 1))^2 + \Delta^2}} \right). \]

Again, the normalization condition is used, and the following is true:
\[ \hat{u}_k^2 = \frac{1}{2} \left( 1 + \frac{\epsilon_k - \lambda + 2\lambda_2(\hat{N} + 1)}{\sqrt{(\epsilon_k - \lambda + 2\lambda_2(\hat{N} + 1))^2 + \hat{\Delta}^2}} \right). \]

Modified pairing gap (\(\hat{\Delta}\)), modified particle number (\(\hat{N}\)), and the new coefficient (\(\lambda_2\)) can be calculated \[76\]. This is done using the following self consistent expressions:

\[ \hat{\Delta} = G \sum_k \tilde{\tau}_k, \]

\[ \hat{N} = 2 \sum_k \tilde{\rho}_k, \]

and

\[ \lambda_2 = \frac{G}{4} \sum_k \frac{(1 - \tilde{\rho}_k)^2 \tilde{\tau}_k \sum_{k'} \tilde{\rho}_{k'} \tilde{\tau}_{k'} - \sum_k (1 - \tilde{\rho}_k)^2 \tilde{\rho}_k^2}{\left( \sum_k (1 - \tilde{\rho}_k) \tilde{\rho}_k \right)^2 - \sum_k (1 - \tilde{\rho}_k)^2 \tilde{\rho}_k^2}. \]

Here, these new compact terms are expressed in terms of SCRPA number projections and BCS coefficients, with:

\[ \tilde{\tau}_k = \hat{u}_k \hat{v}_k \left( 1 - \langle \hat{N}_k \rangle \right), \]

and

\[ \tilde{\rho}_k = \hat{v}_k^2 \left( 1 - \langle \hat{N}_k \rangle \right) + \frac{\langle \hat{N}_k \rangle}{2}. \]

All expressions becomes those of the BCS if \(\lambda_2 = 0\) and \(\langle \hat{N}_k \rangle = 0\). The SCQRPA with LN particle number renormalization is once again be written in
matrix form [63]. However, although this approach is very promising, it has not been applied to isovector pairing. Therefore, the full matrix form will not be included in this discussion. The results for neutrons only are included in Figures A.4 and A.5. A future collaboration may be forged using this technique to allow for the calculation of the terms in the symmetry energy.
Figure A.4. A 14 level calculation of the correlated ground state energy for neutrons as a function of the pairing strength for various approximate approaches compared to the exact solution. The SCQRPA with Lipkin-Nogami values were calculated by Hung [63].
Figure A.5. A 74 level calculation of the correlated ground state energy for neutrons as a function of the pairing strength for various approximate approaches. The breakdown of the RPA solution occurs when the first BCS solution is generated at the critical value of $G = 0.154$. The SCQRPA with Lipkin-Nogami values were calculated by Hung [63].
APPENDIX B

NEW PAIRING APPROACHES

B.1 Hybrid SCRPA and Exact Pairing Solution

A combined approach was developed in order to merge the strengths of two techniques used to describe monopole pairing. Exact calculations involve no approximation. They are solved by means of diagonalization, the dimension which grows quickly. Solutions can only be found using few levels nearest the Fermi surface. SCRPA provides a tool to calculate the pairing for many levels with good agreement with experiment until the critical pairing strength is reached.

The critical pairing strength is known to be dependent on the size of the energy gap at the Fermi surface. The critical pairing strength is increased if the gap is increased. Using an inner exact solution space consisting of a few levels, the critical pairing strength for the SCRPA describing the outer space will be increased.

The number operators of the isovector pairing Hamiltonian included in the SCRPA space are rewritten as boson operators, such that:

\[
H = \sum_{k,\tau} (\epsilon_{k,\tau} - \lambda_{\tau}) N_{k,\tau} - G_{\tau'} \sum_{kk',\tau'} \hat{P}_{k,\tau}^+ \hat{P}_{k',\tau'}^+.
\]

The pair creation and annihilation operators, \((6.7)-(6.9)\), are already bosonic. Commutation relations of interest are as follows:
\[ \langle HF|\hat{P}_{k,-1}, \hat{P}_{k',-1}^+|HF \rangle = \delta_{kk'} (1 - \langle HF|\hat{N}_{k,-1}|HF \rangle), \]

\[ \langle HF|\hat{P}_{k,0}, \hat{P}_{k',0}^+|HF \rangle = \delta_{kk'} \left( 1 - \frac{1}{2} \langle HF|\sum_{\tau} \hat{N}_{k,\tau}|HF \rangle \right), \]

and

\[ \langle HF|\hat{P}_{k,1}, \hat{P}_{k',1}^+|HF \rangle = \delta_{kk'} (1 - \langle HF|\hat{N}_{k,1}|HF \rangle). \]

The isovector hybrid Hamiltonian is of the following form:

\[ H = \sum_{j,\tau} (\epsilon_{j,\tau} - \lambda_{\tau}) \hat{N}_{j,\tau} - G \sum_{j',\tau'} \hat{P}_{j,\tau'}^+ \hat{P}_{j',\tau'} + E_{\text{SCRPA}}^{GSC}, \]

where

\[ E_{\text{SCRPA}}^{GSC} = (\epsilon_m - \lambda) \langle \hat{N}_m \rangle + (\epsilon_i - \lambda) \langle \hat{N}_i \rangle \]

\[ -G \langle \hat{P}_{m}^+ \hat{P}_{m'}^* \rangle + G \langle \hat{P}_{m}^+ \hat{P}_{i}^* \rangle + G \langle \hat{P}_{i}^+ \hat{P}_{m}^* \rangle - G \langle \hat{P}_{i}^+ \hat{P}_{i'}^* \rangle. \]

Here, the full space is denoted by \( k, k' \). The SCRPA space below the Fermi surface is denoted by \( i \), and above the Fermi surface it is \( m \). The small exact subspace nearest the Fermi surface is denoted by \( j, j' \), such that \([k, k'] = [i, j, j', m]\).

This method starts with an uncorrelated ground state. A small subset of the most collective SCRPA phonons is coupled to the exact solutions in the subspace. The collectivity of these phonons was unfortunately not substantially strong, and it seems that the inclusion of many phonons is necessary to find a stable solution. The collectivity of these solutions decreases as the gap near the Fermi surface is increased.
The artificial increasing of a gap in the SCRPA space reduces the coherent strength of the collective excitations. A result of this on the correlated ground state is shown in Figure B.1. It appears as a discrepancy between the results for large pairing strengths. There are two possible solutions to fix this discrepancy. It is possible to rescale the interaction strength. However, attempts to use the BCS to rescale the interaction were unsuccessful. Another possible solution involves including significantly more RPA phonons. It is clear that the latter will not be possible when applied to isovector pairing, because the dimension will become too large.

B.2 Excitation Truncation of Pairing Configurations

The fundamental flaw in using diagonalization to solve pairing problems in nuclei is simply, size. As the number of levels and particles increases, the dimension of the problem grows combinatorially. Although the matrices become increasingly more sparse there is still an eventual limit to the problem caused by hardware limitations, particularly the RAM. The amount of time required for a calculation using traditional diagonalization routines scales as $N^3$ [132]. This means that even if RAM limitations are overcome, the secondary issue of time remains.

Fortunately, it is possible to truncate problems, depending on which observables are of interest. In nuclear physics, this often involves the low energy spectrum which can be compared with experiment. For the cases of evaluating the Wigner X and pairing gap, the ground state with pairing correlations are of interest.

One can calculate the pairing exactly using the levels nearest the Fermi surface. This is known as single particle truncation, and the results of this are shown in Chapter 6. A second technique involves truncating not about a window of the
Figure B.1. Comparison of the hybrid pairing approach compared to SCQRPA with LN particle number renormalization and SCRPA. The Hybrid approaches clearly does not reproduce the same strong correlations for larger pairing strengths. Possible improvements may result from re-normalizing the pairing strength.
single particles, but rather a total energy window based on the sum of over occupied single particle energy. This technique is known as many particle truncation [134].

However, it is also possible to somewhat combine the two approaches such that many levels can be included coming from a few oscillator shells. Few shell calculations are a commonly used choice of basis for pairing calculations [25]. Ground-state calculations can be performed including second order, and on occasion, up to third order excitations with minimal loss of information. This is known as excitation truncation.

The number of configurations \( N \) is based on the combinatorics, where the product of binomial coefficients above and below the Fermi surfaces are calculated. For the generic nucleon pairing, this can be viewed as lifting a number of identical balls from occupied to unoccupied distinguishable levels. The number of excitations \( N_E \) dictates the number of times this is done, and the total number of configurations is written as:

\[
N = \sum_{N_E} \frac{(NL_A)!}{(N_E)!(NL_A - N_E)!} \frac{(NL_B)!}{(N_E)!(NL_B - N_E)!}\]

The number of occupied levels is labeled as \( NL_B = N_{Pairs} \). The number of unoccupied levels is based on the total number of levels \( NL \) such that \( NL_A = NL - NL_B \).

Using this, it is easy to see that there is always one ground state configuration with \( N_E = 0 \). For the case with 20 half filled levels, there will be 100 first order and 2025 second order excitations. The sum of these, together with the previous excitations, are indicated on Figure B.2.

The total number of configurations is based on what comes from the combi-
natorics. This is the same as the previous result when the maximum excitation includes all possible excitations. The sum goes up to the smaller of \(NL_A\) or \(NL_B\), such that:

\[
N = \frac{(NL)!}{(NL_A)!(NL_B)!}.
\]

The principle disadvantage of this approach is that including successive excitations involves calculations with rapidly increasing numbers of configurations. The third order calculation for this 20 level system adds another 14,000+ more configurations with diminishing returns. An alternative means of truncation based on the BCS formalism can be tuned such that a manageable number of configurations is included.

B.3 BCS Truncation of Exact Pairing Configurations

The basic premise is simple for this BCS based truncation. For systems that can be described by the BCS formalism, the wave-function amplitude is largest for configurations most similar to those of the ground state. Specifically, this uses the product \(u_k\) or \(v_k\) for each single particle state in BCS to decide which of the shell model configurations should be kept. If a configuration has a pair on a respective level, then the \(v_k\) is used, otherwise the \(u_k\) is used as defined by (2.32) and (2.33).

A cutoff amplitude and an appropriate choice of \(\Delta\) is then specified. Typically, the use of \(\Delta = 3\) provided good results. The cutoff can then be adjusted such that the desired number of configurations is included. The procedure has the advantage of allowing for the correlations to be calculated as a function of the number of configurations included. This can be used to estimate the correlation for the complete system.
In Figure B.2, it is easy to see that for the system with the gap, the BCS truncation scheme is organized by the order of excitation. The numbers indicated show where each excitation order are included. These show up as corresponding bumps. For systems without substantial gaps in the Fermi surface, the results between using BCS truncation and the excitation truncation differ only slightly. Preference for one opposed to the other varies from case to case.

The method isn’t restricted to calculations of like particles. In fact, an isovector pairing version was developed using a rotated isovector pairing field as described in Section E.3. Moreover, the technique of using an approximate system to determine which configurations are important in an exact calculation is very powerful. Unfortunately, isospin non-conservation, as a function of the cutoff, makes this technique less than optimal for the calculations Wigner X observable.

B.4 Spin Zero Isovector and Isoscalar Pairing

Isoscalar pairing includes modes that are spin aligned \[\text{[37],[121]}\]. This will produce the super-multiplet structure \[\text{[129]}\]. There are six Pauli principle allowed pairs that can be created, as displayed in Figure 6.1 \[\text{[13]}\]. In the strong pairing limit where the pairing strengths are equal, this will result in \(X = 4\) \[\text{[70]}\].

A new isoscalar pairing model was created working under the assumption that the spin aligned modes carry angular momentum and should be largely decoupled from the ground state \[\text{[43]}\]. This means that only one \(T = 0\) state will be allowed with anti-parallel spins. This is can be referred to as the isovector and spin zero isoscalar pairing. In the strong pairing limit of this scheme, with equal isovector \((G)\) and isoscalar \((G_s)\), pairing strengths it will result in \(X = 2\), which is seen in the upper right corner of Figures B.3 and B.4. This seems to be in agreement
Figure B.2. Correlation energy for a system of 20 two-fold degenerate levels systems half filled with like particles, with even level spacing of 1 MeV (green), a pairing strength of .5 MeV, and one with a 5 MeV gap at the Fermi surface (red). The BCS correlation energy is included as a dotted line. Also included are fits which have been extrapolated from the high number dependence up to the full system with 184,756 configurations.
with the experimental fluctuations that average out to a result of $X \approx 2$.

However, it has been demonstrated that isovector pairing alone, with fluctuations caused by shell closures and other deformation related phenomena, explain the Wigner X. The apparent increase in pairing for the $2\Delta$ at $N = Z$, as seen in Figure 6.4 may provide some indication of the isoscalar pairing mechanism. However, it is difficult to decouple this from edge effects caused by the few level calculations.
Figure B.4. Apparent Wigner X for isovector and spin zero isoscalar pairing for a system with six levels, including a substantial energy gap at the $N = Z$ Fermi surface. In the $G_S = 0$ limit the results are the same as those seen with the same level distribution in Figure 6.2.
APPENDIX C

METHODS FOR DETERMINING PROBABILITY DISTRIBUTIONS

C.1 Probability Distribution for Transitional Nuclei from TAC PES

The AutoTAC deformations are found as the lowest point on the PES. Of course, this obscures vital information about how rigid the deformation is and whether there are any low energy secondary or higher order minima.

The conventional picture for shape coexistence comes from transitional nuclei in which there are two competing minima. The pairing interaction used in the AutoTAC calculations will generally smooth the equilibrium deformation between two or potentially more minima. These competing minima are more obvious when examining the unpaired single particle energies. For cases with competing oblate and prolate minima, this may result in a mixed triaxial minima as seen in Figure C.1. However, it is also possible to have multiple minima that are all prolate or oblate. For example, $^{156}$Gd is a case with 11 excited $E_0^+$ states below 3 MeV [3]. Some of these are the result of shape coexistence. The calculation described in Appendix C.2 indicates that an important secondary minimum and equilibrium minimum are both prolate.

The energy difference between the minima is extremely sensitive to the model inputs, such as the single particle level spacing. Results from various models will often disagree with experimental measurements of, for example, the neutron...
Figure C.1. AutoTAC Triaxial ($\gamma$) parameter for Nilsson levels. Nuclei near the colored regions are likely candidates for shape coexistence.
number at which a given isotope will transition from having a well deformed to spherical shape.

A more reasonable approach is to include deformation fluctuations by means of an adiabatic approximation, in which the shape dynamics, such as quadrupole, are assumed to be slow compared to the other excitation modes, such as, the dipole vibrations resulting in the strength functions.

The backward finite difference approximation which uses a discretized function on the given \(x_i(\varepsilon_2)\) grid was used to numerically solve the ensuing differential equation. The kinetic energy can be defined as the change in finite differences among adjacent terms along the grid. PES from TAC are used in the Hamiltonian to describe axial shape fluctuations:

\[
H(x) = \frac{1}{2M} \frac{d^2}{dx^2} + E_{TAC}(x).
\]

After applying the backward finite difference approximation, this Hamiltonian becomes the following:

\[
H(x_i(\varepsilon_2)) = \frac{1}{2M} \left( \frac{x_{i+1}(\varepsilon_2) - 2x_i(\varepsilon_2) + x_{i-1}(\varepsilon_2)}{(\Delta x(\varepsilon_2))^2} \right) + E_{TAC}(x_i(\varepsilon_2)).
\]

Here \(x_i\) is the grid position, \(\Delta x\) is the grid spacing \(\Delta \varepsilon_2 = .15\), and \(M\) is the mass parameter. The mass parameter determines the kinetic energy of the system which for similar nuclei should be smoothly varying.

In Figure C.2, the mass parameter was chosen to be \(M = 100\) in order to best reproduce the experimental \(B(E2)\) from Raman et al. [96]. In this framework, the theoretical \(B(E2)\) can be calculated as the sum products of probabilities for a given deformation, with the \(B(E2)\) for that deformation as calculated in TAC. The severe problem with this approach was the unpredictable \(N-Z\) dependence.
Figure C.2. The probability distribution of $^{98}$Mo as a function of the mass parameter, which adjusts the amount of fluctuations.
Figure C.3. Folded QRPA strength function resulting from the weighted sum of strength functions for various deformations. This combines the differing responses from various deformations of which the nearest to spherical deformations dominate with $-0.15 \leq \varepsilon_2 \leq 0.15$.

of the mass parameter, even for nearby nuclei. The mass parameter required to reproduce the experimental $B(E2)$ varied in a seemingly uncontrollable manner, limiting the predictive power of this approach. This may have been caused by the use of axial deformation parameters for triaxial nuclei.
C.2 Probability Distribution Generated by Configuration Based Deformation Hopping

A new microscopic model for calculating the fluctuations of the nuclear shape was suggested and tested. The isovector pairing Hamiltonian is diagonalized in a basis that consists of multi-pair excitations from the uncorrelated ground state. In contrast to the pairing model used in Chapter 6, the new model allows for the equilibrium deformation to be calculated separately of each configuration by means of the micro-macro method. Information about the structure of the ground state and the lowest excited states can be used to calculate the $B(E2)$ transition probabilities in addition to the probability distribution of shapes present in the ground state.

A shape coexistence code was then created with the intention of allowing each configuration to have an equilibrium deformation based on some slightly course grid. This is very similar to the approach which generated the probability distribution shown in Figure 4.3. The shortcoming of this technique is that collective features are not included in the calculations. Too few states are included to properly smooth out the total potential energy surfaces.

The TAC generates the quadrupole moment ($Q_i$) for a given configuration and the isovector Hamiltonian is diagonalized to calculate pairing correlations and the ground state wave-function. The relative transition probability of a $2^+_\nu$ rotational state based on the excited $0^+_\nu$ state is approximated by the following:

$$B(E2, 2^+_\mu \rightarrow 0^+_\nu) / B(E2, 2^+_1 \rightarrow 0^+_1) = \frac{\langle \mu | \hat{Q} | \nu \rangle^2}{\langle 1 | \hat{Q} | 1 \rangle}.$$

Where $\hat{Q}$ is a diagonal matrix with the values $Q_i$ obtained for each configuration. The eigenstates ($| \mu \rangle$) are the superposition of the uncorrelated configurations
\[ |\mu\rangle = \sum_i c_i^\mu |i\rangle. \]

The scattering of pairs by the monopole pairing interaction makes the pair excitations hop between different shapes. The problem is solved by numerical diagonalization, allowing for protons and neutrons excitations. The combinatorics are the same as those of the Fermi-Hubbard Model for a system of electrons allowed to hop on a lattice [62]. The new hopping model is also analogous to the phenomenon in condensed matter physics of configuration space hopping between meta-stable states in glasses [99]. The configurations that are used are defined by pair excitations on the 6-8 levels nearest to the Fermi surface. The resulting correlated ground state wave-functions give the probability distribution as a function of the deformation for given nucleus. The probability of the nucleus being in a particular deformation is given by the sum over all \(c_i^2\). The sum runs over all deformation parameters on within a given bin interval, defined by \(\Delta \varepsilon_2\) and \(\Delta \gamma\).

Figure C.4 contains the probability distributions generated, which can be compared with the preferred IBM based approach in Figure 4.3.

This procedure depends on tuning the pairing strength parameter. Standard Nilsson levels and a global pairing strength, based on adjacent nuclei, were used for these calculations. The low lying position of \(E_{0^+}\) states in nuclei showing shape coexistence were not well reproduced with this technique, particularly the multitude of low lying \(E_{0^+}\) states seen in \(^{156}\text{Gd}\) [3].

The lower bound for the first excited state, coming in the no pairing limit, is defined by the single particle level spacing. For \(^{156}\text{Gd}\) the single particle spacing was too large.
Figure C.4. Low level pairing calculation ground state probability distribution for Molybdenum. Note that the cell size in the triaxial degree of freedom increases as deformation increase.
Additionally, the $B(E2, 2^+_\mu \rightarrow 0^+_\nu)$ turned out to be too small. Generally, we observe that the collective quadrupole correction seem to be too weak. One possible reason for this is that the few level pairing correlations do not generate significant collective features. Another possibility is that configurations different from the ones considered with zero seniority will be coupled by an interaction of the $Q \cdot Q$ type.

This configuration hopping approach was not successful in reproducing the experimentally observed X. Perhaps this is because the X is too sensitive to the deformation and this approach relies too heavily on the single particle levels. A slight modification of this approach allowed for the evaluation of the observable as a function of a constant deformation for each nucleus, which was used when determining the adopted $\varepsilon_2$ values from Tables 6.2–6.7.
APPENDIX D

ASTROPHYSICAL NUCLEOSYNTHESIS

D.1 Introduction

Primordial Nucleosynthesis is believed to have occurred shortly into the big bang and created mostly deuterium, \(^3\)He, \(^4\)He, and \(^7\)Li. Nuclear burning in the core of a star like our Sun is responsible for the creation of slightly heavier elements. The PP chains, the triple-\(\alpha\) process, CNO cycle, etc. involve stellar burning. Stars more massive than our Sun can fuse nuclei together generating energy and creating elements up to \(^{56}\)Ni or \(^{56}\)Fe at which point fusion will cease because it is no longer profitable energetically. The s-process occurs in stellar environments where the rate of neutron capture is slow relative to the \(\beta^-\)-decay rate, and heavier elements are created along the valley of stability. Supernovae, which generate bursts of energetic particles, are also responsible for the creation of neutron rich elements with masses larger than \(A = 56\). These are the dominant astrophysical processes in which nucleosynthesis occurs.

D.2 Stellar Nucleosynthesis

The nuclear structure material presented in this work, concerns the binding energies of \(N \approx Z\) nuclei and photo-absorption of nuclei far from stability. For
this reason, the specifics on stellar nucleosynthesis of light mass nuclei will only be briefly mentioned.

D.2.1 Stellar Burning

Nucleosynthesis in main sequence stars occurs in a series of phases, in which the star evolves from burning one type of fuel to another. As one fuel becomes depleted the star’s temperature and density will adjust as a result of the lower radiation pressure caused by fewer nuclear reactions occurring in its core. If a star is massive enough it will become so hot and dense in the core that it will eventually begin to fuse together more massive elements. This can occur for stars with approximately one sixteenth the mass of the sun and up to the Eddington mass limit of 120 solar masses \( (M_{\odot}) \) \[20\]. Below this range the gas cannot become hot or dense enough to sustain fusion. Above this the stellar winds will blow the outer layers away.

Depending on the mass of the star, nuclear burning can occur in both the core and shells in which the heavier elements will be produced up to Iron and Nickel. Exotic processes can create neutron rich varieties of these elements.

D.2.2 Late Burning in Massive Stars

If a star is massive enough, with about 8\(+\) \( M_{\odot} \), the light mass nuclear fuel, \(^1\text{H}\) and \(^4\text{He}\), is used up in a star quickly \[100\]. Next, the star will begin to fuse together particles in the intermediate steps of the CNO cycle in the core of the star. This is followed by the burning of neon, sodium, magnesium and if the temperature is high enough silicon, which can also burn combining with a series of seven \(^4\text{He}\) to create \(^{56}\text{Ni}\) \[22\]. Each burning process occurs on increasingly
TABLE D.1

EVOLUTIONARY STAGES OF A 25 M$_\odot$ STAR [128].

<table>
<thead>
<tr>
<th>Stage</th>
<th>Time Scale</th>
<th>Temp. [10$^9$K]</th>
<th>Density [g cm$^{-3}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen Burning</td>
<td>7 x 10$^6$ y</td>
<td>0.06</td>
<td>5</td>
</tr>
<tr>
<td>Helium Burning</td>
<td>5 x 10$^5$ y</td>
<td>0.23</td>
<td>7 x 10$^2$</td>
</tr>
<tr>
<td>Carbon Burning</td>
<td>600 y</td>
<td>0.93</td>
<td>2 x 10$^6$</td>
</tr>
<tr>
<td>Neon Burning</td>
<td>1 y</td>
<td>1.7</td>
<td>4 x 10$^6$</td>
</tr>
<tr>
<td>Oxygen Burning</td>
<td>6 months</td>
<td>2.3</td>
<td>1 x 10$^7$</td>
</tr>
<tr>
<td>Silicon Burning</td>
<td>1 d</td>
<td>4.1</td>
<td>3 x 10$^7$</td>
</tr>
<tr>
<td>Core Collapse</td>
<td>seconds</td>
<td>8.1</td>
<td>3 x 10$^9$</td>
</tr>
<tr>
<td>Core Bounce</td>
<td>milliseconds</td>
<td>34.8</td>
<td>$\approx$ 3 x 10$^{14}$</td>
</tr>
<tr>
<td>Explosive Burning</td>
<td>0.1-10 seconds</td>
<td>1.2-7</td>
<td>varies</td>
</tr>
</tbody>
</table>

shorter time scales as Table [D.1] indicates.

Intermediated mass stars will become Asymptotic Giant Branch (AGB) stars late in their lifetime. In these $^4$He rich stars, the triple $\alpha$ process occurs as well as neutron liberation via ($\alpha$,n) reactions [46]. This causes an increased flux of high energy neutrons, which will allow for neutron rich elements to be created. These elements will then $\beta^-$-decay back toward stability and after some time will absorb more neutrons and $\beta^-$-decay again. This is known as the slow neutron capture process or s-process, which is partially responsible for the creation of elements heavier than $^{56}$Fe.
D.3 Supernovae Nucleosynthesis

There are various phenomena that cause a star to explode as a supernova. Supernovae can generate more exotic nuclei far from the line of stability, because they involve a neutron rich environment near the proto-neutron star. They have been long seen as new stars that appear quickly and fade some within a few months. In the following, the different types of supernova will be discussed. Type I supernovae are missing the characteristic hydrogen lines seen in type II.

D.3.1 Companion Accretion

A type Ia supernova probably involves either a pair of low mass main sequence stars with one accreting material onto another, or a white dwarf that merges with either another white dwarf, or a white dwarf that has another star accreting matter onto its surface. Both processes will increase the temperature and density of the material in the star and it will eventually undergo a thermonuclear explosion of the carbon in the star, creating more and more heavy elements on a much shorter timescale [61]. This explosion will release $10^{10}$ times more energy than is released by our sun over a period of several weeks [53]. Radiation from the material that the explosion has carried away will continue be generated by the radioactive decay of $^{56}$Ni to $^{56}$Co and eventually $^{56}$Fe.

Companion accretion can also result in the rp-process, which will create proton rich nuclei up to the proton drip line. This requires a large flux of high energy protons, such as when a companion star’s outer hydrogen rich envelope falls onto a neutron star. This will be observed as a X-ray burst. It should be noted that the rp-process can be indicated by $(α,p)$ reactions of hot CNO cycle breakout. These nuclei will eventually $β^+$-decay back in toward the valley of stability.

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D.3.2 Core Collapse Supernovae

Type Ib and Ic supernovae occur in more massive stars, which have lost their outer hydrogen and helium envelopes due to either strong solar winds or accretion onto a companion star. The stars that make type II supernovae undergo typical stellar evolution for massive stars and retain their outer envelopes of hydrogen and helium. Core collapse supernovae occur when a Nickel-Iron core has been created in a massive star. As stated before, further fusion will not generate energy, and the radiation pressure of the star will decrease. The outer shells of the star will begin to fall inward. The collapse will continue inward until it has reached nuclear density. As the electron degeneracy pressure is overcome, electrons and protons combine producing neutrons and electron neutrinos which escape the star. This is in part because a substantial amount of matter, about half of it, will re-implode with the remnant [27]. They can interact via neutrino bremsstrahlung, photo-neutrino, and the neutrino Compton effect [26]. One-tenth of the energy of the star is converted into neutrinos which leave the star [100].

There is a large flux of neutrons created by the neutrinos, and the neutron-rich material is carried away by a neutrino energized wind. This may lead to the rapid, or r-process neutron capture nucleosynthesis, which is responsible for the most massive elements that are created far from stability, near the neutron drip line. The neutron fluxes are so great that many neutrons are absorbed into a nucleus before the nucleus can $\beta^-$-decay. Eventually, elements will $\beta$-decay along an isobaric chain toward stability. The exhaustion of the available neutrons limits the extent to which this process takes place [38].
E.1 Solving BCS using Newton’s Method

Newton’s Method was used in solving the BCS equations. Here, we have two equations and two unknowns. The first gives the number of particles:

\[ N = 2 \sum_k v_k^2, \]

with

\[ v_k^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}} \right), \]

and

\[ u_k^2 = \frac{1}{2} \left( 1 + \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}} \right). \]

Here, the amplitudes are normalized with \( u_k^2 + v_k^2 = 1 \). The number of pairs \( N_{\text{Pairs}} = \frac{N}{2} \) is given by:

\[ N_{\text{Pairs}} = \sum_k \frac{1}{2} \left( 1 - \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}} \right). \]

The second equation defines the pairing gap \( \Delta \), with:
\[ \Delta = \frac{G}{2} \sum_{k} \frac{\Delta}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}. \]

It has a trivial solution of \( \Delta = 0 \) below some critical \( G \). The equation for the non-trivial solution can be rewritten in terms of \( G^{-1} \), defined as:

\[ G^{-1} = \frac{1}{G} = \frac{1}{2} \sum_{k} \frac{1}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}. \]

The following partial derivatives needed are all very similar, with:

\[ \frac{\partial N_{Pairs}}{\partial \lambda} = \frac{1}{2} \sum_{k} \frac{\Delta^2}{(\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2})^3}; \]

\[ \frac{\partial N_{Pairs}}{\partial \Delta} = -\frac{1}{2} \sum_{k} \frac{\Delta (\epsilon_k - \lambda)}{(\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2})^3}; \]

\[ \frac{\partial G^{-1}}{\partial \lambda} = \frac{1}{2} \sum_{k} \frac{(\epsilon_k - \lambda)}{(\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2})^3}; \]

and

\[ \frac{\partial G^{-1}}{\partial \Delta} = -\frac{1}{2} \sum_{k} \frac{\Delta}{(\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2})^3}. \]

In Newton’s Approximation the following two statements are true:

\[ N_{Pairs}(\Delta, \lambda) \approx N_{Pairs}(\Delta_0, \lambda_0) + \frac{\partial N_{Pairs}}{\partial \lambda} \delta \lambda + \frac{\partial N_{Pairs}}{\partial \Delta} \delta \Delta, \]

and

\[ G^{-1}(\Delta, \lambda) \approx G^{-1}(\Delta_0, \lambda_0) + \frac{\partial G^{-1}}{\partial \lambda} \delta \lambda + \frac{\partial G^{-1}}{\partial \Delta} \delta \Delta. \]
After some rearranging, there are two equations relating $\delta \Delta$ with $\delta \lambda$ and vice versa, giving the following:

$$\delta \Delta \approx \frac{N_{Pairs}(\Delta, \lambda) - N_{Pairs}(\Delta_0, \lambda_0)}{\frac{\partial N_{Pairs}}{\partial \Delta}} - \frac{\partial}{\partial \Delta} N_{Pairs} \delta \lambda,$$

and

$$\delta \lambda \approx \frac{G^{-1}(\Delta, \lambda) - G^{-1}(\Delta_0, \lambda_0)}{\frac{\partial G^{-1}}{\partial \lambda}} - \frac{\partial}{\partial \lambda} G^{-1} \delta \Delta.$$

By substituting the equations into each other the quantities that will be minimized $\delta \Delta$ and $\delta \lambda$ can be solved for. Substituting some of the previous relations for the partial derivatives, gives the following:

$$\delta \Delta \approx \frac{N_{Pairs}(\Delta, \lambda) - N_{Pairs}(\Delta_0, \lambda_0)}{\frac{\partial N_{Pairs}}{\partial \Delta}} \cdot \frac{\Delta}{\epsilon_k - \lambda} \cdot \frac{G^{-1}(\Delta, \lambda) - G^{-1}(\Delta_0, \lambda_0)}{\frac{\partial G^{-1}}{\partial \lambda}} \cdot \frac{1}{1 - \frac{\Delta^2}{(\epsilon_k - \lambda)^2}},$$

and

$$\delta \lambda \approx \frac{G^{-1}(\Delta, \lambda) - G^{-1}(\Delta_0, \lambda_0)}{\frac{\partial G^{-1}}{\partial \lambda}} \cdot \frac{\Delta}{\epsilon_k - \lambda} \cdot \frac{N_{Pairs}(\Delta, \lambda) - N_{Pairs}(\Delta_0, \lambda_0)}{\frac{\partial N_{Pairs}}{\partial \Delta}} \cdot \frac{1}{1 - \frac{\Delta^2}{(\epsilon_k - \lambda)^2}}.$$

These equations are solved for by a fully self consistent iterative process. When both of these equations are equal to zero, then a minimum has been located, which corresponds to the BCS solution. For best convergence, particularly near the critical G, a reduced one-tenth step was used so as to not overshoot the minimum. This method gives critical points, both minima and maxima. It is for this reason that small steps toward the minimum are necessary; otherwise, the method may locate a second critical point.
E.2 Isovector Pairing Matrix Elements

One subtlety involves a change in the sign of the interaction. It comes about from a phase shift when working out one of the commutation relations. This occurs when fully occupied levels are excited to or from an empty level by a proton-neutron pair. The isovector pairing interaction can be worked out in second quantization. This is done by placing the interaction \(-G_{\tau'} \sum_{kk',\tau'} \hat{P}^+_k \hat{P}^+_{k',\tau'}\) between final and initial states, which are single particle configurations. The pairing of each type of pair is equal and \(G_{\tau'} = G\) is used, such that:

\[
\langle f | \left( - G \sum_{kk',\tau'} \hat{P}^+_k \hat{P}^+_{k',\tau'} \right) | i \rangle.
\]

Figure E.1 shows four excitations which are used to determine the interaction matrix elements. Examples a and b are shown for proton pair excitations and the same results are true if they are switched for neutrons. In addition, the pairing interaction is such that the matrix elements are the same for an excitation and its inverse.

For Example a, the operators are in normal order such that the matrix elements are straightforward, with:

\[
\langle f | \left( - G \sum_{kk',\tau'} \hat{P}^+_k \hat{P}^+_{k',\tau'} \right) | i \rangle
\]

\[
= \langle 0 | \hat{n}_1 \hat{n}_1 \hat{p}_2 \hat{p}_2 \left( - G \sum_{kk',\tau'} \hat{P}^+_k \hat{P}^+_{k',\tau'} \right) \hat{p}_1^+ \hat{p}_1^+ \hat{n}_1 \hat{n}_1 | 0 \rangle
\]

\[
= -G \langle 0 | \hat{n}_1 \hat{n}_1 \hat{p}_2 \hat{p}_2 \left( \hat{p}_1^+ \hat{p}_1^+ \hat{p}_1 \hat{p}_1 \right) \hat{p}_1^+ \hat{p}_1^+ \hat{n}_1 \hat{n}_1 | 0 \rangle
\]

\[
= -G.
\]
Figure E.1. Four isovector pairing excitation scenarios from which all interactions can be built.
The same is true for Example b, with:

$$
\langle f \bigg| \left( -G \sum_{kk',\tau'} \hat{P}^{+}_{k,\tau'} \hat{P}^{+}_{k',\tau'} \right) \bigg| i \rangle
= \langle 0 \bigg| \hat{p}_2 \hat{p}_2 \left( -G \sum_{kk',\tau'} \hat{P}^{+}_{k,\tau'} \hat{P}^{+}_{k',\tau'} \right) \hat{p}_1 \hat{p}_1 \bigg| 0 \rangle
= -G \langle 0 \bigg| \hat{p}_2 \hat{p}_2 \left( \hat{p}_2 \hat{p}_1 \hat{p}_1 \right) \hat{p}_1 \hat{p}_1 \bigg| 0 \rangle
= -G.
$$

For Example c, the expectation value is the following:

$$
\langle f \bigg| \left( -G \sum_{kk',\tau'} \hat{P}^{+}_{k,\tau'} \hat{P}^{+}_{k',\tau'} \right) \bigg| i \rangle
= \langle 0 \bigg| \frac{1}{\sqrt{2}} \left( \hat{n}_2 \hat{p}_2 + \hat{p}_2 \hat{n}_2 \right) \left( -G \sum_{kk',\tau'} \hat{P}^{+}_{k,\tau'} \hat{P}^{+}_{k',\tau'} \right) \frac{1}{\sqrt{2}} \left( \hat{n}_1 \hat{p}_1 + \hat{p}_1 \hat{n}_1 \right) \bigg| 0 \rangle
= -G \langle 0 \bigg| \frac{1}{\sqrt{2}} \left( \hat{n}_2 \hat{p}_2 + \hat{p}_2 \hat{n}_2 \right) \left( \frac{1}{\sqrt{2}} \left( \hat{n}_2 \hat{p}_2 + \hat{p}_2 \hat{n}_2 \right) \frac{1}{\sqrt{2}} \left( \hat{n}_1 \hat{p}_1 + \hat{p}_1 \hat{n}_1 \right) \right) \frac{1}{\sqrt{2}} \left( \hat{n}_1 \hat{p}_1 + \hat{p}_1 \hat{n}_1 \right) \bigg| 0 \rangle
= -4G/4.
$$

However, for Example d, there is a sign change, such that:

$$
\langle f \bigg| \left( -G \sum_{kk',\tau'} \hat{P}^{+}_{k,\tau'} \hat{P}^{+}_{k',\tau'} \right) \bigg| i \rangle
= \langle 0 \bigg| \frac{1}{\sqrt{2}} \left( \hat{n}_1 \hat{p}_1 + \hat{p}_1 \hat{n}_1 \right) \frac{1}{\sqrt{2}} \left( \hat{n}_2 \hat{p}_2 + \hat{p}_2 \hat{n}_2 \right) \left( -G \sum_{kk',\tau'} \hat{P}^{+}_{k,\tau'} \hat{P}^{+}_{k',\tau'} \right) \hat{p}_1 \hat{p}_1 \hat{n}_1 \hat{n}_1 \bigg| 0 \rangle
= -G \langle 0 \bigg| \frac{1}{\sqrt{2}} \left( \hat{n}_1 \hat{p}_1 + \hat{p}_1 \hat{n}_1 \right) \frac{1}{\sqrt{2}} \left( \hat{n}_2 \hat{p}_2 + \hat{p}_2 \hat{n}_2 \right) \bigg| 0 \rangle
$$
\[ \times \left( \frac{1}{\sqrt{2}} (\hat{n}_2^+ \hat{p}_2^- + \hat{p}_2^+ \hat{n}_2^-) \right) \frac{1}{\sqrt{2}} (\hat{n}_1 \hat{p}_1 + \hat{p}_1 \hat{n}_1) \left( \hat{p}_1^+ \hat{p}_1^+ \hat{n}_1^+ |0\rangle \right) \\
= 4G/4. \]

Ultimately, the minus sign or phase flip comes about from the following:

\[ \hat{p}_k^+ \hat{p}_k^- \hat{n}_k^+ \hat{n}_k^- = -\frac{1}{\sqrt{2}} \left( \hat{n}_k^+ \hat{p}_k^- + \hat{p}_k^+ \hat{n}_k^- \right) \frac{1}{\sqrt{2}} \left( \hat{n}_k^+ \hat{p}_k^- + \hat{p}_k^+ \hat{n}_k^- \right) \cdot \]

The same phase flip occurs for the isoscalar pairing where the proton neutron operator is

\[ \frac{1}{\sqrt{2}} \left( \hat{n}_k^+ \hat{p}_k^- - \hat{p}_k^+ \hat{n}_k^- \right). \]

E.3 Rotations of the Isovector Pair Field

The squared terms of isospin and angular momentum operators are Casimir invariants of the three-dimensional (iso)rotational group \([17]\). The Wigner \(D(\alpha, \beta, \gamma)\) function performs a transformation of states under rotations of the coordinate system. This will be used to rotate from isolated proton and neutron states, used in standard BCS calculations, into states that also include a mixed proton neutron isovector state. A procedure similar to this is commonly used when transforming from angular momentum projection \((M)\) to that of a new coordinate system \(M'\) \([101]\). The following discussion will perform a rotation of the isovector pairing field from the isospin projection \((T_z)\) along the \(\hat{x}\) axis to a new projection \(T_z'\) in the \(\hat{y}-\hat{z}\) plane, with:

\[ D^{(i)}(\alpha, \beta, \gamma) = e^{iT_z'\gamma} D^{(i)}_{T_z', T_z}(\beta) e^{iT_z\alpha}. \]

Here for spin one-half fermions, protons and neutrons, the Wigner \(D^{(1/2)}_{T_z', T_z}(\beta)\) function is the following:
The procedure begins with the combined proton and neutron BCS wavefunctions used to describe an even-even nucleus, with $i$ pairs of neutrons and $j$ pairs of protons:

$$|BCS\rangle = \prod_{i,j} (u_i + v_i \hat{n}_i^+ \hat{n}_i^+)(u_j + v_j \hat{p}_j^+ \hat{p}_j^+)|0\rangle.$$  

The rotated wave-function then takes the form of the expression below:

$$|BCS'\rangle = \prod_{i,j} \left( u_i + v_i \left( \cos(\theta/2)e^{i\pi/4} \hat{n}_i^+ + \sin(\theta/2)e^{i\pi/4} \hat{p}_i^+ \right) \right) \times \left( \cos(\theta/2)e^{i\pi/4} \hat{n}_i^+ + \sin(\theta/2)e^{i\pi/4} \hat{p}_i^+ \right) \times \left( u_j + v_j \left( -\sin(\theta/2)e^{i\pi/4} \hat{n}_j^+ + \cos(\theta/2)e^{i\pi/4} \hat{p}_j^+ \right) \right) \times \left( -\sin(\theta/2)e^{i\pi/4} \hat{n}_j^+ + \cos(\theta/2)e^{i\pi/4} \hat{p}_j^+ \right) \left( -\sin(\theta/2)e^{i\pi/4} \hat{n}_j^+ + \cos(\theta/2)e^{i\pi/4} \hat{p}_j^+ \right) |0\rangle.$$
Figure E.2. The rotation of the isospin pairing field with Euler angles.
The following trigonometric relations will be used for simplification:

\[
\sin^2\left(\frac{\theta}{2}\right) = \frac{1}{2}\left(1 - \cos(\theta)\right),
\]

\[
\cos^2\left(\frac{\theta}{2}\right) = \frac{1}{2}\left(1 + \cos(\theta)\right),
\]

and

\[
\cos\left(\frac{\theta}{2}\right) \sin\left(\frac{\theta}{2}\right) = \frac{1}{2}\left(\sin(\theta)\right).
\]

After applying these, the final rotated wave-function was calculated, giving the following:

\[
|BCS'\rangle = \prod_{i,j} \left( u_i u_j + v_i v_j 
- \frac{i}{2} u_i v_j \left( (1 - \cos(\theta)) \hat{n}_i^+ \hat{n}_i^+ \right) 
+ \frac{i}{2} v_i u_j \left( (1 + \cos(\theta)) \hat{n}_i^+ \hat{n}_i^+ \right) 
- \frac{i}{2} u_i v_j \left( (1 + \cos(\theta)) \hat{p}_i^+ \hat{p}_i^+ \right) 
+ \frac{i}{2} v_i u_j \left( (1 - \cos(\theta)) \hat{p}_i^+ \hat{p}_i^+ \right) 
+ \frac{i}{2} u_i v_j \left( (\sin(\theta))(\hat{n}_i^+ \hat{p}_i^+ + \hat{p}_i^+ \hat{n}_i^+) \right) 
+ \frac{i}{2} v_i u_j \left( (\sin(\theta))(\hat{n}_i^+ \hat{p}_i^+ + \hat{p}_i^+ \hat{n}_i^+) \right) \right)|0\rangle.
\]

Here the angle \(\theta\) is defined in the following way:
\[
\theta = \begin{cases} 
\pi/2, & \text{if } T_z = 0 \\
\frac{1}{\sqrt{T_z}}, & \text{otherwise}
\end{cases}.
\]

For nuclei with significantly different numbers of protons and neutrons this solution returns to the commonly used separate proton-proton and neutron-neutron pairing, because \(\frac{1}{\sqrt{T_z}}\) is small. The phase factors \((\pm i)\) are ignored because the calculations are equivalent in the \(\hat{x}-\hat{y}\) plane.
BIBLIOGRAPHY


