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Electromagnetic Sum Rules and Response Functions from the Symmetry-Adapted No-Core Shell Model

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ELECTROMAGNETIC SUM RULES
AND RESPONSE FUNCTIONS
FROM THE SYMMETRY-ADAPTED
NO-CORE SHELL MODEL

A Dissertation
Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
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Doctor of Philosophy

in
The Department of Physics & Astronomy

by
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B.S. Physics, Austin Peay State University, 2013
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Abstract

Recent developments in \textit{ab initio} nuclear structure have provided us with a variety of many-body methods capable of describing nuclei into the medium-mass region of the chart of nuclides. One of these, the symmetry-adapted no-core shell model (SA-NCSM), capitalizes on inherent symmetries of the nucleus and is uniquely suited to examine the underlying physics of dynamical quantities, such as the response function.

We examine the applicability of the SA-NCSM to calculations of these quantities and assess the quality of its inputs by calculating electromagnetic sum rules and response functions with the Lanczos sum rule method and Lanczos response function method, respectively. Our systematic analysis of $^4$He shows good agreement in the sum rules between the SA-NCSM and hyperspherical harmonics, an exact method. We also detail a novel use of a projection technique to remove spurious center-of-mass contributions to our sum rules. Our calculations for the response functions of $^4$He, $^{16}$O, and $^{20}$Ne reveal the advantages of the SA-NCSM when examining giant resonances and we detail a straightforward procedure to calculate the compressibility of nuclear matter from only the microscopic calculations of these response functions.

The results of this work illustrate the ability of the SA-NCSM to reliably and accurately calculate electromagnetic sum rules, as well as its usefulness in providing physically-informed interpretations of electromagnetic response functions. This suggests future work with the SA-NCSM could provide valuable insights, particularly for open-shell nuclei beyond the reach of other methods.
1 Introduction

Theoretical nuclear physics seeks to describe, and in some cases predict, the properties of a nucleus from the fundamental interactions of the protons and neutrons. This goal encompasses both its structural properties and its dynamical properties, such that we are tasked with knowing both what a nucleus looks like (e.g. What are its eigenstates? What excitation energies can it have? Can we identify any inherent clustering?) and how it will behave (e.g. what happens if we hit it with a beam of protons? How energetic does a photon need to be before it can break the nucleus apart?). The problems posed by this overarching goal can be formidable, though the advent of supercomputers has allowed for considerable progress to be made in the past few decades. With the introduction of realistic interactions derived from first principles and the continued development of robust many-body techniques, nuclear theory is poised to provide precise descriptions of atomic nuclei for both the purposes of gaining a better understanding of the nucleus itself and for being able to provide accurate descriptions of the nucleus as input for other branches of physics.

To better understand the nucleus itself, *ab initio* (or from first principles) methods can model properties of nuclei from the fundamental nucleon-nucleon interaction. This allows us to see connections between the underlying quark-gluon dynamics and the emergence of clustering or collectivity without assuming its existence *a priori*. This can provide insight into the essential ingredients necessary to properly capture descriptions of nuclei. These essential ingredients can then be propagated forward, so that we can use them to describe how a nucleus reacts across a wide range of energies. For example, the next generation of neutrino detectors will require the best possible descriptions of the nuclei that make up their detectors in order to properly model how the neutrino is interacting [1]. As this interaction can take place across a wide range of possible energies, a wide variety of nuclear processes can contribute. A good description of the nuclear response, informed by the essential ingredients to capture the necessary physics, can assist in this process. The goal of this dissertation is to study the applicability of symmetry-adapted no-core shell model (SA-NCSM) wave functions
to these problems (clustering, collectivity, modeling nuclear responses) – in other words, we investigate whether our method, the SA-NCSM, can address these issues from a consistent, symmetry-informed framework.

In Chapter 2, we provide an overview of nuclear shell models, starting from the emergence of shell structure and progressing all the way to the development of the SA-NCSM. We also review the range of nuclear interactions that have been developed and discuss the Lanczos algorithm, a powerful method for solving the eigenvalue problem, to which references will appear throughout the text. In Chapter 3, we detail the physics of response functions for both photoabsorption and electron scattering and discuss techniques for calculating them based on properties of integral transforms. We also introduce sum rules, which are the energy-moments of the response function, and discuss how they can provide valuable information about the response function while also being easier to calculate. Chapter 4 provides, in detail, the results of a benchmark study that illustrates the reliability and accuracy of the SA-NCSM to be able to calculate electromagnetic sum rules in $^4$He [2]. This chapter also details a novel use of a procedure to remove spurious contributions of the center-of-mass, which may have applications in other modern-day nuclear structure techniques. Chapter 5 illustrates the ability of the SA-NCSM to calculate electromagnetic response functions in nuclei beyond the reach of some other techniques, including the open-shell nucleus $^{20}$Ne [3]. We also examine these response functions for signatures of giant resonances, which are collective excitations involving most, if not all, of the nucleons. We connect properties of these giant resonances to the compressibility of infinite nuclear matter. Lastly, Chapter 6 summarizes these findings.
2 Nuclear Shell Models

The atomic nucleus is a complicated many-particle system to study and describe theoretically. While a large number of approaches have been employed, with varying degrees of success, one persistent theme to emerge from experimental data was the existence of shell structure. In particular, this can be seen through the regular changes in nuclear properties around the “magic numbers” which correspond to closed shells of neutrons and protons [4,5]. This behavior is analogous to the changes in atomic properties around closed shells for electrons in atomic physics and chemistry. While we a priori might not expect a system of strongly-interacting particles to be well described by their interactions with a mean field that they themselves create, subsequent research found it to work fairly well. In this chapter, we will follow a semi-historical progression from the traditional nuclear shell model to the modern implementation of the symmetry-adapted no-core shell model.

2.1 The nuclear Hamiltonian

In principle, the nuclear many-body Hamiltonian used to describe $A$ point-like non-relativistic strongly-interacting nucleons reads

$$H = \sum_i \frac{\vec{p}_i^2}{2m} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots,$$

(2.1)

where $m$ is the mass of a nucleon, $\vec{p}_i$ is the momentum of the $i$-th particle, and $V_{ij}$ and $V_{ijk}$ are two-nucleon (NN) and three-nucleon (NNN) interaction terms. As nucleons themselves are composite particles composed of quarks and gluons, higher-body interactions could also be included in this Hamiltonian, but their inclusion will not be discussed here. Note that this Hamiltonian includes the center-of-mass motion, which will be discussed in detail below. Additionally, given the success of nuclear theory in describing experimental data without including these higher-body interactions, it is generally believed that their effects must be quite small.
2.1.1 Independent particle model

Focusing on the NN interaction, $V_{ij}$, the traditional shell model is able to reproduce the magic numbers by decomposing this into a mean field interaction and an (assumed) negligible residual interaction characterizing the remaining two-body effects. This looks like

$$\sum_{i<j}^{A} V_{ij} = \sum_{i}^{A} V_{i} + \sum_{i<j}^{A} V_{\text{res}}^{ij}, \quad (2.2)$$

where $V_{i}$ is a mean field. The approach is often called the independent particle model (IPM), as it treats each nucleon separately and allows them to independently interact with the average potential created by the remaining nucleons. In this way, we can write the nuclear Hamiltonian as a sum over single-particle Hamiltonians

$$H = \sum_{i}^{A} \left( \frac{\vec{p}_{i}^2}{2m} + V_{i} \right) = \sum_{i}^{A} H_{i}. \quad (2.3)$$

In this approximation, each particle behaves independently and we have reduced the complicated many-body problem into a problem where we need only solve the Schrödinger equation for the single-particle energies and wave functions. That is, we are solving

$$H_{i} \psi_{\alpha}(\vec{r}_{i}) = E_{i}^{\alpha} \psi_{\alpha}(\vec{r}_{i}), \quad (2.4)$$

where $\psi_{\alpha}(\vec{r}_{i})$ and $E_{i}^{\alpha}$ are the single-particle wave functions and energies, respectively. Here, $\alpha$ represent the quantum numbers relevant to the single-particle state and $\vec{r}_{i}$ are the single-particle coordinates. Should we choose the familiar harmonic oscillator (HO) potential $V_{\text{HO}}(\vec{r}_{i}) = \frac{1}{2} m \Omega^2 \vec{r}_{i}^2 = \frac{m \Omega^2}{2} \left( \frac{\vec{r}_{i}}{b} \right)^2$, where $b = \sqrt{\frac{\hbar}{m \Omega}}$ is the harmonic oscillator length parameter,
then the resulting wave functions are

$$\psi_\alpha(x, y, z) = \langle x, y, z|n_x n_y n_z m_s \rangle = H_{n_x}(x)H_{n_y}(y)H_{n_z}(z) \exp\left(-\frac{m\Omega(x^2 + y^2 + z^2)^2}{2\hbar}\right) \chi_{\frac{1}{2}m_s}$$

(2.5)

in Cartesian coordinates, where $H_{n_i}$ are the Hermite polynomials, $\chi_{\frac{1}{2}m_s}$ is the standard spinor for spin-$\frac{1}{2}$ particles, and our $\alpha = (n_x, n_y, n_z, m_s)$. The $n_i$ describe excitations of a nucleon in the $i$-th direction ($i = x, y, z$) and $m_s$ is the spin projection of the nucleon ($m_s = -\frac{1}{2}, \frac{1}{2}$). In spherical coordinates, this would instead look like

$$\psi_\alpha(r, \theta, \phi) = \langle r, \theta, \phi|\eta \ell m_l m_s \rangle = N_{\eta \ell} R_{\eta \ell}(r) Y_{\ell m_l}(\theta, \phi) \chi_{\frac{1}{2}m_s},$$

(2.6)

where $Y_{\ell m_l}(\theta, \phi)$ are the spherical harmonics, $N_{\eta \ell}$ is a normalization factor, and the radial wave function, $R_{\eta \ell}(r)$, is given by

$$R_{\eta \ell}(r) = r^\ell \exp\left(-\frac{r^2}{2b^2}\right) L_{(\eta - l)/2}^{l + \frac{1}{2}} \left(\frac{r^2}{b^2}\right).$$

(2.7)

Here, $L_{(\eta - l)/2}^{l + \frac{1}{2}} \left(\frac{r^2}{b^2}\right)$ are generalized/associated Laguerre polynomials. In this basis, our $\alpha = (\eta, l, m_l, m_s)$, where $\eta$ is the HO shell number ($\eta = 0, 1, 2, 3, \ldots$ for the $s, p, sd, pf, \ldots$ shells), $l$ is the orbital angular momentum ($l = \eta, \eta - 2, \ldots, 1$ or 0), $m_l$ is the $z$-projection of the orbital angular momentum, and $m_s$ is the same as before.

While the wave functions may look different depending on our choice of coordinate system, the energies (which is an observable) must be independent of this choice. As such, either choice yields energies of

$$E_N = \hbar \Omega \left(N + \frac{3}{2}\right).$$

(2.8)

For the Cartesian case $N = n_x + n_y + n_z$ and for the spherical case $N = \eta$. 

5
Each single-particle state carries its own quantum numbers and comprises a complete and orthonormal basis in the Hilbert space. Respecting nucleons as the fermions they are, then the many-body wave function will be an antisymmetrized product of the single-particle wave functions. A convenient way to write this many-body wave function is with a Slater determinant such that

\[ \Psi_{\alpha\beta...\omega}(\vec{r}_1, \vec{r}_2, ..., \vec{r}_A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \psi\alpha(\vec{r}_1) & \psi\alpha(\vec{r}_2) & \cdots & \psi\alpha(\vec{r}_A) \\ \psi\beta(\vec{r}_1) & \psi\beta(\vec{r}_2) & \cdots & \psi\beta(\vec{r}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \psi\omega(\vec{r}_1) & \psi\omega(\vec{r}_2) & \cdots & \psi\omega(\vec{r}_A) \end{vmatrix}. \]  

(2.9)

Note that for historical accuracy, the HO potential alone is insufficient to reproduce the magic numbers. Instead one must use

\[ V_i = V_{\text{HO}} + V_{\text{spin-orbit}} + V_{\text{orbit-orbit}} \]

\[ = \frac{1}{2} m \Omega^2 r_i^2 - \alpha \vec{l}_i \cdot \vec{s}_i - \beta l_i^2 \]  

(2.10)  

(2.11)

where the constants \( \alpha \) and \( \beta \) can tune the strength of the spin-orbit and orbit-orbit interactions, respectively. Solving the resulting Schrödinger equation yields the experimentally observed magic numbers 2, 8, 20, 28, 50, 82, . . . .

### 2.1.2 Nuclear interactions

While certainly instructive, the IPM is unable to capture much of the physics of nuclei, especially for open-shell nuclei which are not near one of the magic numbers corresponding to closed shells. As such, a more complete theoretical description must allow for non-negligible residual interactions – or equivalently, a nucleon-nucleon interaction that cannot be approximated by a mean field. Keeping in mind the lessons from the IPM, we need not start from scratch. For example, since the IPM can describe closed shell nuclei fairly well, we could
allow these more complicated NN interactions to apply to only the valence nucleons, i.e. the nucleons which sit above the closed shell. This approach treats all of the other (core) nucleons as “inactive,” meaning that they cannot interact with the valence nucleons. This is the idea behind the valence shell model. In such an approach, one usually truncates shells higher than the valence shell. This truncation restricts the states that can be described to ones of the same parity and thus would not be able to provide a complete description of atomic nuclei.

2.2 No-core shell model

Building on the idea of an interacting shell model, we can unfreeze the nucleons in the core and allow for every nucleon to be excited to any given shell. This is the idea behind the no-core shell model (NCSM) [6], which underpins the concepts discussed in the remainder of this chapter. Recalling the nuclear Hamiltonian from before

$$H = \frac{1}{A} \sum_{i<j}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j}^{A} V_{ij}$$

(2.12)

where we have kept only up to the NN terms and made the kinetic energy translationally invariant. Now that every nucleon is active, we must also have an adequate way of describing how they are configured in our model space so that we can classify each configuration in a consistent way. This is usually done by keeping track of the number of harmonic oscillator quanta $N$ above the ground state configuration in the model space. For example, in the ground state configuration of $^4$He the two protons and two neutrons completely fill the $\eta = 0$ or $s$ shell. An $N = 2$ configuration allows for two more HO quanta to be introduced, thereby exciting a nucleon up two shells or two nucleons up one shell. If we only allow configurations with $N = 2$ in our model space, this is called an $N_{\text{max}} = 2$ truncation and this allows us to partition our otherwise infinite model space into a series of finite subspaces. A schematic representation of some possible configurations allowed in the $N_{\text{max}} = 2$ model space of $^4$He is shown in Fig. 2.1. As we have artificially introduced this truncation scheme, any calculations
we perform in this approach must be independent of the choice of $N_{\text{max}}$. With this framework in mind, any NCSM calculation requires two additional points of discussion: the basis and the interaction.

![Diagram of two possible configurations of $^4\text{He}$ in the $N_{\text{max}} = 2$ model space.](image)

**Figure 2.1**: A schematic representation of two possible configurations of $^4\text{He}$ in the $N_{\text{max}} = 2$ model space. On the left, one particle has been moved up two shells and on the right two particles have been moved up one shell.

### 2.2.1 The basis

Recalling our spherical coordinate wave function from before, and neglecting spin, we know a single nucleon can be described with $\psi_{nlm}(\vec{r}) = R_{nl}(r)Y_{lm}(\theta, \phi)$, where $\vec{r}$ describes the position of this nucleon in the chosen coordinate system with an implicitly chosen origin point. As we start including more nucleons, we must describe their positions with other vectors $\vec{r}_i$, and we have a choice for how to do this. Either we describe the position of each subsequent nucleon in relation to the previous ones (Jacobi coordinates) or we describe the position of each subsequent nucleon with respect to a common point (laboratory-frame coordinates).

For Jacobi coordinates, the basis is labeled according to $\vec{\xi}_i$, where $i$ corresponds to the coordinate number and not the particle number. The first Jacobi coordinate is the distance between particle 1 and particle 2 such that

$$\vec{\xi}_1 = \sqrt{\frac{1}{2}}(\vec{r}_1 - \vec{r}_2).$$

(2.13)
Each subsequent $\vec{\xi}_i$ coordinate is then defined in relation to the positions of the center-of-mass of the preceding particles such that

$$\vec{\xi}_2 = \sqrt{\frac{2}{3}} \left( \frac{1}{2} [\vec{r}_1 + \vec{r}_2] - \vec{r}_3 \right),$$

(2.14)

or more generally

$$\vec{\xi}_{j-1} = \sqrt{\frac{j-1}{j}} \left( \frac{1}{j-1} \left[ \sum_{i=1}^{j-1} \vec{r}_i \right] - \vec{r}_j \right),$$

(2.15)

where $j = 2, \ldots, A$. A schematic of what these coordinates look like is shown in Fig. 2.2. While keeping track of only relative coordinates does allow us to avoid any issues with the center-of-mass, it becomes intractable to construct many-body wave functions in relative coordinates for more than $A = 7$ particles. This is because our many-body wave functions must be antisymmetric with respect to particle interchange and the antisymmetrization process is impossible beyond $A = 7$. Nonetheless, this coordinate system has been employed in a number of nuclear theory calculations, including in implementations of the NCSM with a Jabobi basis [7] and in the hyperspherical harmonics (HH) approach [8].

Figure 2.2: (a) An illustration of the Jacobi coordinates defined by Eqs. (2.13-2.15). (b) An illustration of laboratory coordinates.
For laboratory-frame coordinates, we allow each position vector to originate from some implicitly chosen origin, as shown in Fig. 2.2. Since physics must be independent from the coordinate system we choose to work in, this artificially introduces spurious center-of-mass states which describe the motion of the center-of-mass of the nucleus and not the intrinsic states of the nucleus that we are interested in. With the HO basis, we are able to exactly separate the intrinsic states of a nucleus from the spurious center-of-mass states, even in the $N_{\text{max}}$ truncation scheme [9]. With laboratory-frame coordinates, we can continue to use the previously described Slater determinant method to construct many-body wave functions that are antisymmetric with respect to particle exchange. In this approach, the many-body wave functions will look like

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{R}) = \psi_{\text{intrinsic}}(\vec{r}_1, \vec{r}_2, \ldots) \psi_{\text{CM}}(\vec{R}),$$

where $\psi_{\text{intrinsic}}(\vec{r}_1, \vec{r}_2, \ldots)$ represents the intrinsic state of the nucleus and $\psi_{\text{CM}}(\vec{R})$ represents the center-of-mass state, dependent on the center-of-mass position $\vec{R} = \frac{1}{A} \sum_{i=1}^{A} \vec{r}_i$. Since we are only interested in these intrinsic states, and not in excitations of the center-of-mass, we must always ensure the center-of-mass wave function is in its ground state. In the language of the HO quantum numbers before, this would be $\alpha = (\eta = 0, l = 0, m_l = 0)$. In practical applications, this can be guaranteed through the use of the Gloeckner-Lawson projection method [10]. This requires us to add another term to the Hamiltonian, $\lambda H_{\text{CM}}$, where $\lambda$ is a Lagrange multiplier and $H_{\text{CM}}$ is the center-of-mass Hamiltonian

$$H_{\text{CM}} = \frac{\vec{P}^2}{2mA} + \frac{1}{2} Am\Omega^2 \vec{R}^2.$$  

(2.17)

Here, $\vec{R}$ is the center-of-mass position and $\vec{P}$ is the center-of-mass momentum $\vec{P} = \sum_{i=1}^{A} \vec{p}_i$. In its original form, the Lawson term is added to the $A$-body Hamiltonian $H_A$ such that

$$H = H_A + \lambda \left( H_{\text{CM}} - \frac{3}{2} \hbar \Omega \right),$$

(2.18)
where the second term in parenthesis subtracts off the energy of the three-dimensional HO in its ground state. Thus, for a many-body wave function with the center-of-mass in the ground state \( \lambda (H_{\text{CM}} - \frac{3}{2} \hbar \Omega) \psi_{\text{CM},000} = 0 \), whereas any other center-of-mass state will be excited to higher in the energy spectrum by a value of \( \lambda \). With a sufficient large value of \( \lambda \), we can cleanly separate the relevant intrinsic states from the spurious center-of-mass states.

### 2.2.2 The interaction

While the strong force is available from quantum chromodynamics (QCD), it is non-perturbative at the low energy scales relevant to nuclear structure. This fact has led to many techniques to construct a nuclear interaction that can be used to model, and potentially predict, nuclear properties. While not the primary focus of this work, here we will briefly discuss some of the terms used to describe the resulting interactions, including schematic, empirical, and realistic interactions.

Some interactions are fully schematic interactions, meaning they assume a usually simple form for the nuclear interaction and adjust some number of parameters to reproduce experimental data. The chosen forms are often based on known properties of the nuclear force, e.g. given that the nuclear force is short range, one could choose a short range function such as a delta function and see how well it describes known properties. More complicated forms can also be chosen, such as one involving the quadrupole operator \([11–13]\) as will be discussed later in this chapter.

Some nuclear interactions are empirical, in that they do not assume an underlying functional form, but instead adjust the value of the nuclear matrix elements to experimentally known nuclear data \([14]\). These are often constructed in the context of the shell model and are restricted to a given valence space, e.g. the \(pf\) shell.

The last class of interactions is dubbed realistic because they are able to reproduce nucleon-nucleon scattering data (primarily phase shifts up to a certain energy cutoff) with a reduced \( \chi^2 \sim 1 \) \([15,16]\). In general, they are also required to reproduce the properties
of the deuteron exactly [17]. For three-body forces, they are often required to reproduce the properties of $^3$H and/or $^3$He. Nuclear structure calculations performed with these realistic interactions are generally referred to as “ab initio,” or from first principles. These requirements do not imply a specific technique to construct such an interaction, and in fact a good number of techniques can be used to make realistic interactions. For example, interactions based on meson-exchange potentials, e.g. CD-Bonn [18] and Argonne [19], can be realistic, and interactions derived from an underlying chiral effective field theory ($\chi$EFT) can also be realistic interactions. As such, ab initio calculations tend to involve the use of multiple realistic interactions, derived from multiple techniques, such that the differences in the interactions when used to study a particular phenomenon can be readily identified, and potentially addressed in the next generation of realistic interactions.

With this in mind, we will now briefly discuss more details of the realistic interactions used in this work. This includes the JISP16 potential and two potentials derived from chiral effective field theory.

**JISP16 potential**

The JISP16 potential is based on the $J$-matrix inverse scattering potential approach [20], which first derives a nucleon-nucleon interaction and then performs a unitary transformation to improve its description of excitation spectra in the $p$ shell and better reproduce the deuteron quadrupole moment. This unitary transformation is phase-equivalent and does not alter its designation as realistic. The JISP16 interaction does include fits to the excitation energies of $^6$Li and the binding energies of $^6$Li and $^{16}$O, and is generally only designed to work for $A \leq 16$ nuclei. JISP16 is also known to be a relatively “softer” interaction, meaning that it converges relatively quickly with respect to the expansion parameter $N_{\text{max}}$. 
Chiral interactions

In an attempt to derive nuclear interactions from the underlying quark-gluon dynamics inherent in QCD, effective field theories can be employed [21]. In this way, one can construct a Lagrangian from chiral EFT that describes the nucleons in a nucleus interacting via pion exchange. The Feynman diagrams describing these interactions introduce low-energy constants, which can be determined from experimental data or perhaps one day from QCD itself.

An important feature of $\chi$EFT is its perturbative nature. That is, at each higher order of the $\chi$EFT Lagrangian we gain another power of our expansion parameter, and can thus guarantee that higher order terms will contribute less than lower order terms. This hierarchy reflects the previously mentioned fact that higher body forces (e.g. 4N forces) don’t contribute on the same level as two body (NN) forces.

Of particular note here are the N3LO-EM [22] and NNLO$_{opt}$ [23] potentials. The N3LO-EM interaction is based off of the original Entem and Machleidt derivation, which kept NN terms up to the next-to-next-to-next-to leading order. Here, we have used only the NN interaction and have not implemented the 3N interactions. The NNLO$_{opt}$ potential keeps NN terms up to the next-to-next-to leading order and is optimized to reduce the need for 3N interactions.

For the sake of completeness, it is necessary to mention that N3LO-EM is known to be an interaction with a comparatively hard core, which means that it does not converge very quickly with respect to $N_{\max}$. This requires one of the two following approaches: either one must go to high $N_{\max}$ to show the necessary model space convergence, or one must “soften” the interaction in some way. A good number of renormalization techniques exist to soften interactions, e.g. Okobo-Lee-Suzuki (OLS), similarity renormalization group (SRG), and others. We have not used renormalization techniques in this work for a few reasons. First, as will be discussed toward the end of this chapter, the symmetry-adapted no-core shell model (SA-NCSM) has a unique ability to reach larger model spaces than other methods,
thereby reaching the necessary convergence with $N_{\text{max}}$. Second, using a renormalization procedure changes the details of the Hamiltonian, thus also changing the details of the resulting wave functions. To calculate an observable with these wave functions, one must also renormalize the operator in the same way. While such renormalization has been carried forward, albeit truncated at a low order, collective observables remain difficult to reproduce. In the SA-NCSM, we eliminate the need for such renormalization. It is important to note that the SA-NCSM has a unique ability to examine the contributions of intrinsic deformation to the many-body wave functions. A renormalized interaction would change these individual contributions in ways that would preclude our standard analysis of the wave functions in terms of these intrinsic deformations.

### 2.2.3 Implementing the NCSM

Any discussion of the NCSM is incomplete without also discussing how to solve the resulting large-dimensional eigenvalue problem. Recall that our main goal is to solve the basic eigenvalue problem of

$$H\Psi = E\Psi,$$  \hspace{1cm} (2.19)

where $H$ is the many-body Hamiltonian we have now constructed in the chosen basis with the chosen nuclear interaction, $\Psi$ is the unknown many-body wave function, and $E$ is the unknown energy describing the state $\Psi$. Here, we have elected to use $H$ and $\Psi$ to emphasize these are the matrix and vector forms of the Hamiltonian and wave function. The number of basis states (or the dimensionality of the Hamiltonian matrix) for NCSM calculations can easily grow to millions (or possibly billions) very quickly and we are left to solve for the eigenvalues and eigenvectors of that matrix. Luckily, nuclear structure generally only cares about the lowest eigenvalues and eigenvectors for each system and as a result many NCSM practitioners implement the Lanczos algorithm [24].
In its extreme form, the Lanczos algorithm is a procedure to determine the unitary matrix $Q$ which turns a real, symmetric, $N \times N$ matrix $H$ into an $N \times N$ tridiagonal matrix $T$ such that

$$Q^T H Q = T,$$

where $T$ denotes the transpose (since $H$ is real, $Q$ will also be real so taking the complex conjugate will be unnecessary) [25]. Generally, the columns of $Q$ are denoted as $q_i$ and are called a Lanczos basis – they constitute an orthonormal basis of $H$. A complete description of the Lanczos procedure is outlined in Fig. 2.3 [26]. After constructing this tridiagonal matrix $T$, we can use a simple tridiagonal matrix solver to find its eigenvalues, which will correspond to the eigenvalues of $H$.

In this extreme form, the Lanczos algorithm is just a matrix diagonalization procedure. However, the advantage of the Lanczos procedure is that it does not have to be iterated the full $N$ times to create the $N \times N$ matrix, $T$. Instead, we can stop iterating at some $k$, where

---

Figure 2.3: Pseudocode for the Lanczos algorithm. Note $H$ is our $N \times N$ matrix of interest, $Q$ is a $N \times k$ matrix whose columns are composed of the Lanczos basis vectors $q_i$, the vectors $x, r, v$ are all of length $N$, and $\alpha$ and $\beta$ are the elements of the tridiagonal matrix $T_{k}$. 

```
1: pick $x$
2: $q_0 = \frac{x}{||x||}$ Q_{:,0} = q_0
3: $r = Hq_0$
4: $\alpha_0 = q_0 \cdot r$
5: $r = r - \alpha_0 q_0$
6: $\beta_0 = ||r||$
7: for $k = 1, 2, \ldots$
8: $v = q_k$ $q_k = \frac{r}{\beta_{k-1}}$ Q_{:,k} = q_k
9: $r = Hq_k - \beta_{k-1} v$
10: $\alpha_k = q_k \cdot r$
11: $r = r - \alpha_k q_k$
12: $\beta_k = ||r||$
```
\[ k \leq N, \text{ and construct some } k \times k \text{ matrix that looks like} \]

\[
T_k = \begin{pmatrix}
\alpha_0 & \beta_1 & 0 & 0 & \ldots & 0 & 0 \\
\beta_1 & \alpha_1 & \beta_2 & 0 & \ldots & 0 & 0 \\
: & : & : & \ddots & \vdots & : & : \\
0 & 0 & 0 & 0 & \ldots & \alpha_{k-2} & \beta_{k-1} \\
0 & 0 & 0 & 0 & \ldots & \beta_{k-1} & \alpha_{k-1}
\end{pmatrix}.
\] \tag{2.20}

Should we then apply a tridiagonal matrix solver to this matrix, we will find that the eigenvalues of this smaller \( k \times k \) matrix rapidly converge to the extreme (the highest and the lowest) eigenvalues of \( H \) [26]. Since the NCSM only needs the lowest-lying states, the Lanczos process is well-suited to solve for those eigenvalues and eigenvectors.

As a clarifying note, recognize that the algorithm described in Fig. 2.3 provides the tridiagonal matrix elements \( \alpha \) and \( \beta \) that are needed to construct \( T_k \). As stated above, the \( k \) possible eigenvalues of \( T_k \) will correspond to the extreme eigenvalues of \( H \). The eigenvectors of \( T_k \), here denoted as \( s_i \), can be used to construct the eigenvectors of \( H \), \( y_i \), as

\[ y_i = Q_k s_i. \]

Note that on the \( k \)th iteration, the matrix \( Q \) will be of size \( N \times k \) and the eigenvector of \( T \) will be of length \( k \). Thus the matrix-vector multiply will yield \( y_i \) with length \( N \) – a necessary requirement for an eigenvector of \( H \) since it is of dimensions \( N \times N \).

### 2.3 Symmetry-informed approach

Even with the advantages of modern-day computing, NCSM calculations tend to encounter a scale explosion problem. This means that the size of the basis grows combinatorially with larger \( N_{\text{max}} \), and so calculations can and do become impossible to perform, even on the best available supercomputers today. The scale explosion problem is illustrated in Fig. 2.4.
Figure 2.4: Dimension of the model space for the ground state of various nuclei as a function of $N_{\text{max}}$. As can be seen, the size of the model space grows quickly with respect to $N_{\text{max}}$.

To be able to use the NCSM as nuclear theory expands to higher mass ranges, a number of approaches have been developed. These range from applications of perturbation theory [27] to implementations of Monte Carlo techniques [28], but here we will focus on the use of inherent symmetries in nuclear physics, in particular the symplectic symmetry [29–31] and the no-core symplectic shell model (NCSpM) [13, 32]. The NCSpM is based on the physically-relevant symplectic $Sp(3,\mathbb{R})$ group and uses symplectic basis states, which are unitary transformations of the many-body basis states used in standard NCSM calculations. The original implementation of the NCSpM uses a schematic interaction based on the quadrupole-quadrupole interaction and is able to reproduce the properties of the Hoyle state, a feat that has only been accomplished by preliminary calculations by the ab initio Lattice EFT using the best realistic interactions [33]. This fact strongly hints at the importance of the symplectic symmetry to nuclear structure and serves as the impetus to the development of the symmetry-adapted no-core shell model to be discussed next.
2.3.1 Symmetry-adapted no-core shell model

The symmetry-adapted no-core shell model (SA-NCSM) takes advantage of the underlying, emergent symplectic symmetry present in nuclei to decrease computational demands and better our ability to describe nuclei beyond the lightest species with realistic interactions [34, 35]. Specifically, its collective basis is composed of an equilibrium deformation, characterized by the quantum numbers \((\lambda \mu)\) illustrated in Fig. 2.5, plus vibrations and rotations of that deformation. Like other no-core shell models, it utilizes an \(N_{\text{max}}\) truncation to systematically control the growth of the model space.

Figure 2.5: Illustrations of different \((\lambda \mu)\) configurations, where each corresponds to a different deformation.

The SA-NCSM differs from other approaches in its ability to control the growth of the model space by including only the physically-relevant basis states. Previous results have shown that realistic interactions display an underlying symplectic symmetry (see Fig. 2.6 and Refs. [34, 35]) and the SA-NCSM is uniquely designed to take advantage of this. Our symmetry-adapted approach is illustrated in Fig. 2.7.

Of particular relevance here is the underlying symplectic symmetry inherent in the SA-NCSM. For example, giant resonances, which are collective excitations of the nucleons and will be discussed in more detail in the following chapters, are incorporated in the symplectic symmetry – the vibrations of the equilibrium deformation include them and in fact they are created by one of the generators of the symplectic group [30]. Thus, the SA-NCSM is uniquely suited for studies of these giant resonances from an \textit{ab initio} perspective.
Figure 2.6: A breakdown of the $^6$Li ground state wave function produced from the JISP16 interaction in an $N_{\text{max}} = 10$ model space. Each column corresponds to $(\lambda \mu)$ configuration probability in the wave function. The diagonal lines represent the projection of the full wave function onto one symplectic irrep, e.g. for the red line, 80% of the full ground state wave function project onto a single symplectic irrep. Figure adapted from Ref. [34].
Figure 2.7: Schematic depiction of the symmetry-adapted approach. Top row: We allow the particles to fill the lowest possible states in the harmonic oscillator potential and allow excitations up to some $N_{\text{max}}$. As can be seen in the bottom portion of the top row, this approach includes portions of the model space (the area inside the box) that do not contribute to the nucleus. The symmetry-adapted approach can be used as a guide when discarding those physically-irrelevant portions, thereby freeing up computational resources to perform higher $N_{\text{max}}$ calculations. Bottom row: When we expand this picture to higher $N_{\text{max}}$ spaces, we introduce vibrations of our equilibrium deformation that can extend beyond the original model space. By varying the number of states included in these higher spaces (the size of the extra boxes on the model space), we can show convergence.
3 Response Functions and Integral Transforms

3.1 Response functions

3.1.1 Photoabsorption

First, we will discuss the details of photoabsorption reactions since the response function for this case is fairly straightforward and will serve as a good conceptual starting point for further discussion. In a photoabsorption reaction, a single photon of some energy is absorbed by the nucleus, which causes the nucleus to transition to a final state different from its initial state. This process is represented by the diagram in Fig. 3.1. There, a single photon $\gamma$ interacts with the initial state of the nucleus $|\psi_i\rangle$, is absorbed, and causes the nucleus to transition to a final state $|\psi_f\rangle$. Note the spread of the lines on the final state indicates that a variety of possible outgoing channels are available, including states in which the initial nucleus breaks up into fragments.

![Figure 3.1: A schematic diagram describing the photoabsorption process where a single photon $\gamma$ is absorbed by the nucleus.](image)

A characteristic photonuclear response (or cross section) is shown in Fig. 3.2. If the energy $\omega$ of the incoming photon is low, we can see the excitation of individual discrete states in the nucleus. As the energy increases, we can see a broad resonance. This type of resonance is known as a giant resonance and it corresponds to collective motion involving many, if not all, of the nucleons. Further increases in the energy will lead to the $\Delta$-resonance, which is the excitation of an individual nucleon.
Figure 3.2: The characteristic response (or cross section) of a photoabsorption process as a function of energy transfer.

To describe photoabsorption, the cross section can be parameterized as

$$\sigma_\gamma(\omega) = 4\pi^2 \alpha \omega R(\omega),$$

where $$\alpha = \frac{1}{137}$$ is the fine-structure constant and

$$R(\omega) = \sum_f \left| \left< \psi_f \left| \hat{D} \right| \psi_i \right> \right|^2 \delta (E_f - E_i - \omega)$$

is the dipole response function and $$\hat{D}$$ is the dipole operator [36].

### 3.1.2 Electron scattering

Increasing the complexity, we will discuss response functions in the context of electron scattering. An electron inelastically scattering off of a nucleus, e.g. as shown in Fig. 3.3, in the Born approximation will exchange a virtual photon and the final state of the nucleus will be different from the initial state.

A characteristic response for inelastic electron scattering is shown in Fig. 3.4. While many of the same features from photoabsorption are retained (discrete excited states, giant resonances, $$\Delta$$-resonance), for inelastic electron scattering we have another continuum resonance known as the quasi-elastic peak. This peak around $$\omega = q^2/2m$$ corresponds to electrons scattering off of single nucleons [37].
Figure 3.3: A schematic diagram describing an electron scattering off of a nucleus through the exchange of a single photon $\gamma$, with (a) showing the particle labels and (b) indicating the four-momenta.

Figure 3.4: The characteristic response of electron scattering as a function of energy transfer.

The double-differential cross section for this reaction is then

$$
\frac{d^2\sigma}{d\Omega_e d\omega} = \sigma_M \left( \frac{(q^2 - \omega^2)^2}{q^4} R_L(\omega, q) + \left[ \frac{q^2 - \omega^2}{2q^2} + \tan^2 \left( \frac{\theta_e}{2} \right) \right] R_T(\omega, q) \right) \tag{3.3}
$$

where $q = |\vec{q}|$, and

$$
\sigma_M = \left( \frac{\alpha \cos \left( \frac{\theta_e}{2} \right)}{2\epsilon \sin^2 \left( \frac{\theta_e}{2} \right)} \right)^2 \tag{3.4}
$$

is the Mott cross section, which describes electron scattering off of a point-like nucleus [36]. The electron initial energy and scattering angle are given by $\epsilon$ and $\theta_e$, respectively. Given the appearance of the Mott cross section in Eq. 3.3, it is clear the terms in the parenthesis on the right hand side must correspond to corrections arising from the underlying nuclear structure, since the nucleus is not point-like. These terms are the longitudinal (L) and transverse (T)
response functions and for this process the longitudinal one is defined as

$$R_L(\omega, q) = \sum_f \left| \langle \psi_f | \rho(\vec{q}) | \psi_i \rangle \right|^2 \delta \left( E_f - E_i - \omega + \frac{\vec{q}^2}{2M_A} \right), \quad (3.5)$$

where $|\Psi_i\rangle$ and $|\Psi_f\rangle$ are the initial and final states of the nucleus with energies $E_i$ and $E_f$, respectively, and $\rho(\vec{q})$ is the charge density. The symbol $\sum_f \int f$ reflects the fact we must sum over all possible final states, including the discrete (sum) ones and the continuum (integral) ones. The last term in the energy-conserving $\delta$-function recognizes that the nucleus (with mass $M_A$) could recoil during this reaction. Similarly, the transverse response function is given by

$$R_T(\omega, q) = \sum_f \sum_{\lambda=\pm1} \left| \langle \psi_f | J_\lambda(\vec{q}) | \psi_i \rangle \right|^2 \delta \left( E_f - E_i - \omega + \frac{\vec{q}^2}{2M_A} \right), \quad (3.6)$$

where the operator is now the electromagnetic current $J_\lambda(\vec{q})$ and we must sum over the allowed polarizations $\lambda$ of the virtual photon.

In this situation (inelastic electron scattering), no real photons are involved and so the momentum and energy transfers can vary independently. This requires $R_L$ and $R_T$ to be functions of both. This is in contrast to photoabsorption, which involves real photons, and so the response function could only depend on the energy transfer $\omega$.

As mentioned previously, these response functions must carry all of the relevant nuclear structure information, which they do via the wave functions. However, the sum over all possible final states complicates the direct calculations of a response function since it requires nuclear structure theorists to have excellent descriptions of every state in a nuclear energy spectrum, including states in the continuum. As many nuclear structure calculations rely on bound-state techniques, e.g. the HO basis in the NCSM, a proper description of the continuum can be challenging and thus most response functions are not calculated directly.
3.2 Integral transforms

As mentioned, a direct calculation of a response function is generally beyond the reach of current techniques due to the requirement that all states in the excitation spectrum be well described. It is worthwhile to note that this does not just refer to continuum states and their necessary asymptotics being beyond the scope of many bound-state techniques, but it also refers to the fact that a nucleus could break up into smaller fragments and one would also need good descriptions of those channels. Thus, one of the often used techniques to avoid this complication is the use of an integral transform of the form

\[ I(\sigma) = \int d\omega K(\sigma, \omega) R(\omega), \]  

(3.7)

where \( K(\sigma, \omega) \) is a-yet-to-be-defined kernel that maps the information in the response function \( R(\omega) \) to a new function \( I(\sigma) \). A Fourier transform is a standard example of such a procedure, where the idea is that we can transform into a different function/representation and it will be easier to perform calculations with that function than with the original function. This means that we need to be able to calculate the integral transform \( I(\sigma) \) easier than we can calculate \( R(\omega) \).

It is worth noting that it can be difficult to assign any physical meaning to the integral transform itself. However, as can be seen from Fig. 3.5, a kernel approximating a \( \delta \)-function has the beneficial advantage of reproducing our response function in such a way that we can still assign physical interpretations to its peaks. There, we have folded and example response function with a Lorentzian of the form

\[ K(\sigma, \omega) = \frac{1}{(\omega - \sigma)^2 + \Gamma^2} \]  

(3.8)

and in the limit of \( \Gamma \rightarrow 0 \), the Lorentzian becomes a \( \delta \)-function. However, direct use of a
$\delta$-function as the kernel in Eq. 3.7 would not gain us much as

$$I(\sigma) = \int d\omega \delta(\omega - \sigma) R(\omega) = R(\sigma)$$

(3.9)

and so we would not have succeeded in finding an integral transform that is easier to calculate than the response function.

![Figure 3.5: (a) An example of a response function and (b) the integral transform of it for different values of the width $\Gamma$ of the Lorentzian given by Eq. (3.8).](image)

In the subsections that follow, we will discuss a couple of the kernels that have been employed, or continue to be employed, in calculations for the response function. These will include only the Stieltjes kernel and the Lorentz kernel, though other kernels have been used by other groups [38,39].

### 3.2.1 Stieltjes transform

The Stieltjes kernel looks like

$$K(\sigma, \omega) = \frac{1}{\omega + \sigma},$$

(3.10)

where $\sigma$ is a real, positive number [40]. Negative values of $\sigma$ will introduce poles in our transform since the energy transfer $\omega$ will be positive. If we plug this kernel and the general
expression for the response function into Eq. (3.7), we find

\[ I(\sigma) = \int d\omega \frac{R(\omega)}{\omega + \sigma}. \]  

(3.11)

Substituting for the definition of the response function, we find

\[ I(\sigma) = \sum \int d\omega \left| \langle \psi_f | \hat{O} | \psi_i \rangle \right|^2 \frac{\delta(E_f - E_i - \omega)}{\omega + \sigma}. \]  

(3.12)

\[ = \sum \int \frac{\left| \langle \psi_f | \hat{O} | \psi_i \rangle \right|^2}{E_f - E_i + \sigma}, \]  

(3.13)

where we have used the \( \delta \)-function to integrate over \( \omega \). If we now rewrite the numerator,

\[ I(\sigma) = \sum \int \langle \psi_i | \hat{O}^\dagger | \hat{\Psi}_f \rangle \langle \psi_f | \hat{O} | \psi_i \rangle \frac{1}{E_f - E_i + \sigma}. \]  

(3.14)

\[ = \sum \int \langle \psi_i | \hat{O}^\dagger \left( \frac{1}{\hat{H} - E_i + \sigma} \right) | \psi_f \rangle \langle \psi_f | \hat{O} | \psi_i \rangle. \]  

(3.15)

\[ = \langle \psi_i | \hat{O}^\dagger (\hat{H} - E_i + \sigma)^{-1} \hat{O} | \psi_i \rangle, \]  

(3.16)

where we have substituted the final energy \( E_f \) with the Hamiltonian \( \hat{H} \) according to the relation \( \hat{H} | \Psi_f \rangle = E_f | \Psi_f \rangle \) and then invoked completeness of the final states \( 1 = \int | \psi_f \rangle \langle \psi_f | \). This rearrangement makes it clear that the primary ingredients to calculating the integral transform are the operator \( \hat{O} \) for the problem at hand, the Hamiltonian \( \hat{H} \), and the initial state energy \( E_i \) and wave function \( | \psi_i \rangle \). Thus, any bound state technique should be able to yield good descriptions of this integral transform. Issues arise when trying to invert this transform and recover the response function [41]. As has been shown in previous work [42], the process suffers numerical issues in the higher energy ranges and cannot be used satisfactorily to calculate the responses at an arbitrary energy without significant care being taken.

It is worthwhile to note that even though the inversion is complicated, the Stieltjes
transform itself is straightforward and can be useful. An example of this is the electric dipole polarizability $\alpha_D$, which can be calculated with the Stieltjes transform and the coupled-cluster method. The electric dipole polarizability is defined as

$$\alpha_D = 2\alpha \int d\omega \frac{R(\omega)}{\omega}. \quad (3.17)$$

Comparing this expression to Eq. 3.11, we can see that $\sigma$ is the only difference under the integrand. Thus, if we take $\lim_{\sigma \to 0^+}$, we can calculate the electric dipole polarizability without calculating the full response, i.e.

$$\alpha_D = 2\alpha \lim_{\sigma \to 0^+} I(\sigma). \quad (3.18)$$

This has been done quite successfully [43, 44].

**3.2.2 Lorentz transform**

As mentioned above, the Lorentz kernel is given by

$$K(\sigma, \omega) = \frac{1}{(\omega - \sigma)^2 + \Gamma^2}, \quad (3.19)$$

where $\Gamma$ is the width of the Lorentzian centered around $\sigma$ [41]. Repeating the same process we did for the Stieltjes kernel, we find

$$I(\sigma) = \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} \quad (3.20)$$

$$= \sum_f \frac{\langle \psi_i | \hat{O}^\dagger | \psi_f \rangle \langle \psi_f | \hat{O} | \psi_i \rangle}{(E_f - E_i - \sigma)^2 + \Gamma^2} \quad (3.21)$$

$$= \sum_f \frac{1}{(\hat{H} - E_i - \sigma)^2 + \Gamma^2} \langle \psi_f | \hat{O} | \psi_i \rangle \quad (3.22)$$

$$I(\sigma) = \langle \psi_i | \hat{O}^\dagger \frac{1}{(\hat{H} - E_i - \sigma)^2 + \Gamma^2} \hat{O} | \psi_i \rangle. \quad (3.23)$$
If we recognize the denominator as the square of a complex number

\[(E_f - E_i - \sigma)^2 + \Gamma^2 = (E_f - E_i - \sigma + i\Gamma)(E_f - E_i - \sigma - i\Gamma),\]  

(3.24)

then we can equivalently write

\[I(\sigma) = \langle \psi_i | \hat{O}^\dagger(\hat{H} - E_i - \sigma + i\Gamma)^{-1}(\hat{H} - E_i - \sigma - i\Gamma)^{-1}\hat{O}|\psi_i \rangle \]  

(3.25)

\[I(\sigma) = \langle \Psi'|\Psi' \rangle, \]  

(3.26)

where, if we assume \(\hat{O}^\dagger = \hat{O}\),

\[|\Psi'\rangle = (\hat{H} - E_i - \sigma - i\Gamma)^{-1}\hat{O}|\psi_i \rangle \]  

(3.27)

Rewriting Eq. (3.20) like this implies that solving for the integral transform \(I(\sigma)\) is akin to solving a Schrödinger-like equation with a source term

\[(\hat{H} - E_i - \sigma - i\Gamma)|\Psi'\rangle = \hat{O}|\psi_i \rangle.\]  

(3.28)

To solve for the integral transform \(I(\sigma)\) in an efficient way, we must first do one more rearrangement. If we start from the quantity

\[\text{Im}\left[\langle \psi_i | \hat{O}^\dagger(\hat{H} - E_i - \sigma - i\Gamma)^{-1}\hat{O}|\psi_i \rangle\right], \]  

(3.29)

and rationalize the denominator such that

\[\text{Im}\left[\langle \psi_i | \hat{O}^\dagger \frac{1}{\hat{H} - E_i - \sigma - i\Gamma}\hat{O}|\psi_i \rangle\right] = \text{Im}\left[\langle \psi_i | \hat{O}^\dagger \frac{\hat{H} - E_i - \sigma + i\Gamma}{(\hat{H} - E_i - \sigma)^2 + \Gamma^2}\hat{O}|\psi_i \rangle\right]\]  

(3.30)

\[= \Gamma\langle \psi_i | \hat{O}^\dagger \frac{1}{(\hat{H} - E_i - \sigma)^2 + \Gamma^2}\hat{O}|\psi_i \rangle.\]  

(3.31)
We can immediately recognize this righthand side as $\Gamma$ multiplied by Eq. (3.23). Thus,

$$I(\sigma) = \frac{1}{\Gamma} \text{Im} \left[ \langle \psi_i | \hat{O}^\dagger \frac{1}{\hat{H} - E_i - \sigma - i\Gamma} \hat{O} | \psi_i \rangle \right].$$  \hspace{1cm} (3.32)

If we set $z = E_i + \sigma + i\Gamma$ and define a normalized vector

$$|\phi_0\rangle = \frac{\hat{O}|\psi_i\rangle}{\sqrt{\langle \psi_i | \hat{O}^\dagger \hat{O} | \psi_i \rangle}} ,$$  \hspace{1cm} (3.33)

then we can write

$$I(\sigma) = -\frac{1}{\Gamma} \langle \psi_i | \hat{O}^\dagger \hat{O} | \psi_i \rangle \text{Im} \left[ \langle \phi_0 | \frac{1}{z - \hat{H}} | \phi_0 \rangle \right] .$$  \hspace{1cm} (3.34)

Now, this is where the Lanczos algorithm reappears. If we recognize the term inside the imaginary brackets as a matrix element

$$x_{00} = \langle \phi_0 | \frac{1}{z - \hat{H}} | \phi_0 \rangle$$  \hspace{1cm} (3.35)

and treat $|\phi_0\rangle$ as the pivot vector in our Lanczos algorithm, then we can define a Lanczos basis $\{|\phi_n\rangle\}$. From here, we can start with the identity $(z - \hat{H})(z - \hat{H})^{-1} = 1$, such that

$$(z - \hat{H})(z - \hat{H})^{-1} = 1$$  \hspace{1cm} (3.36)

$$(z - \hat{H})(z - \hat{H})^{-1}|\phi_0\rangle = |\phi_0\rangle$$  \hspace{1cm} (3.37)

$$(z - \hat{H}) \sum_n |\phi_n\rangle \langle \phi_n | (z - \hat{H})^{-1} |\phi_0\rangle = |\phi_0\rangle$$  \hspace{1cm} (3.38)

$$\sum_n \langle \phi_m | (z - \hat{H}) |\phi_n\rangle \langle \phi_n | (z - \hat{H})^{-1} |\phi_0\rangle = \langle \phi_m | \phi_0 \rangle$$  \hspace{1cm} (3.39)

$$\sum_n (z - \hat{H})_{mn} x_{n0} = \delta_{m0},$$  \hspace{1cm} (3.40)
which defines a matrix equation. To solve it, we can invoke Cramer’s rule \[45\]

\[ x_{00} = \frac{\det[(z - \hat{H})_0]}{\det[(z - \hat{H})]} \]

(3.41)

where \( \det[...] \) is the determinant and \( \det[(z - \hat{H})_i] \) is the determinant of the \( (z - \hat{H}) \) matrix when the \( i \)-th column has been replaced by the column vector on the righthand side of Eq. (3.40). Recall the application of the Lanczos algorithm in Eq. (2.20) produces a symmetric tridiagonal Hamiltonian of the form

\[
T_k = \begin{pmatrix}
\alpha_0 & \beta_1 & 0 & 0 & \ldots & 0 & 0 \\
\beta_1 & \alpha_1 & \beta_2 & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \ldots & \alpha_{k-2} & \beta_{k-1} \\
0 & 0 & 0 & 0 & \ldots & \beta_{k-1} & \alpha_{k-1}
\end{pmatrix}
\]

Thus, after some algebra we can rewrite Eq. (3.41) as

\[
x_{00} = \frac{\det[B]}{(z - \alpha_0)\det[B] - \beta_1\det[B_1]} \\
= \frac{1}{z - \alpha_0 - \beta_1 \frac{\det[B_1]}{\det[B]}},
\]

(3.42) (3.43)

where

\[
B = \begin{pmatrix}
(z - \alpha_1) & \beta_2 & 0 & 0 & \ldots & 0 & 0 \\
\beta_2 & (z - \alpha_2) & \beta_3 & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \ldots & (z - \alpha_{k-2}) & \beta_{k-1} \\
0 & 0 & 0 & 0 & \ldots & \beta_{k-1} & (z - \alpha_{k-1})
\end{pmatrix}
\]

(3.44)
and

\[
B_1 = \begin{pmatrix}
\beta_1 & \beta_2 & 0 & 0 & \ldots & 0 & 0 \\
0 & (z - \alpha_2) & \beta_3 & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \ldots & (z - \alpha_{k-2}) & \beta_{k-1} \\
0 & 0 & 0 & 0 & \ldots & \beta_{k-1} & (z - \alpha_{k-1})
\end{pmatrix}.
\] (3.45)

This process is recursive, such that continued applications of Cramer's rule leads to a continued fraction of the form

\[
x_{00} = \frac{1}{(z - \alpha_0) - \frac{\beta_2^2}{(z - \alpha_1) - \frac{\beta_3^2}{(z - \alpha_2) - \frac{\beta_4^2}{\ddots}}}}.
\] (3.46)

In this way, provided we start with an appropriate pivot vector, we can use the Lanczos coefficients from the many-body calculation to calculate the Lorentz integral transform as

\[
I(\sigma) = -\frac{1}{\Gamma} \langle \psi_i | \hat{O}^\dagger \hat{O} | \psi_i \rangle \text{Im} \left[ \frac{1}{(z - \alpha_0) - \frac{\beta_2^2}{(z - \alpha_1) - \frac{\beta_3^2}{(z - \alpha_2) - \frac{\beta_4^2}{\ddots}}}} \right].
\] (3.47)

With this quantity in hand, we can either invert it to recover the response function, or as illustrated with Fig. 3.5, choose an appropriate value of the width \( \Gamma \) and investigate the physics from there.

### 3.3 Sum rules

In some cases, it is either not possible to calculate the response function or too expensive to calculate the response function via any current methods. However, that does not prevent us from learning information about the response function indirectly. This is primarily done through calculating the energy moments of the response function, which are otherwise known.
as sum rules. It worth noting that since the response function is related to the cross section through some kinematic factors, it is often easier to probe the sum rule from experimental data than it is to probe the response function from experimental data. Sum rules can be extracted from experimental data often by integrating over the cross section, which is an easier procedure than extracting the response function directly. As such, we will now discuss a straightforward and efficient technique to calculate sum rules with an arbitrary energy weighting.

Consider the general response function

\[ R(\omega) = \sum \int f |\langle \psi_f | \hat{O} | \psi_i \rangle|^2 \delta(E_f - E_i - \omega), \]  

(3.48)

where \( \hat{O} \) is a generic operator describing a transition. With this, we can define a sum rule with an arbitrary energy weighting as

\[ m_n = \int d\omega R(\omega)\omega^n, \]  

(3.49)

where \( n \) can be any real number that does not have to be an integer. Substituting for the response function, we find

\[ m_n = \int d\omega \sum \int f |\langle \psi_f | \hat{O} | \psi_i \rangle|^2 \delta(E_f - E_i - \omega)\omega^n \]  

(3.50)

\[ = \sum \int f |\langle \psi_f | \hat{O} | \psi_i \rangle|^2 (E_f - E_i)^n \]  

(3.51)

\[ m_n = \sum |\langle \psi_\mu | \hat{O} | \psi_i \rangle|^2 (E_\mu - E_i)^n, \]  

(3.52)

where in the last step, we have assumed we will be employing bound-state techniques to solve for the final states \( |\psi_\mu \rangle \), and thus we do not need to integrate over the continuum states [46].

From the discussion of the Lanczos algorithm before, we know that we can construct a
tridiagonal matrix $T$ representing the Hamiltonian $H$ as

$$
\hat{H} = QTQ^T,
$$

(3.53)

where $Q$ is unitary matrix that performs the transformation. With the Lanczos basis states denoted by $|\phi_k\rangle$, then the eigenstates of our Hamiltonian $|\psi_n\rangle$ after $N$ Lanczos iterations are given by

$$
|\psi_n\rangle = \sum_{k=0}^{N-1} Q_{kn} |\phi_k\rangle.
$$

(3.54)

If we substitute this equation into the sum rule expression given by Eq. (3.52), then

$$
m_n = \sum_{\mu} \left| \sum_{k=0}^{N-1} Q_{k\mu}^T \langle \phi_k | \hat{O} | \psi_i \rangle \right|^2 (E_{\mu} - E_i)^n.
$$

(3.55)

Recalling our definition of the pivot vector $|\phi_0\rangle = \hat{O} |\psi_i\rangle / \sqrt{\langle \psi_i | \hat{O}^\dagger \hat{O} | \psi_i \rangle}$, then

$$
m_n = \langle \psi_i | \hat{O}^\dagger \hat{O} | \psi_i \rangle \sum_{\mu} \left| \sum_{k=0}^{N-1} Q_{k\mu}^T \langle \phi_k | \phi_0 \rangle \right|^2 (E_{\mu} - E_i)^n
$$

(3.56)

$$
= \langle \psi_i | \hat{O}^\dagger \hat{O} | \psi_i \rangle \sum_{\mu} \left| \sum_{k=0}^{N-1} Q_{k\mu}^T \delta_{k0} \right|^2 (E_{\mu} - E_i)^n
$$

(3.57)

$$
= \langle \psi_i | \hat{O}^\dagger \hat{O} | \psi_i \rangle \sum_{\mu} |Q_{\mu0}|^2 (E_{\mu} - E_i)^n,
$$

(3.58)

where we have used the fact that the Lanczos basis is orthonormal to evaluate the inner sum. Thus, similar to the case with the Lorentz integral transform, we can see that to evaluate a sum rule with an arbitrary energy weighting we only require knowledge of the initial state $|\psi_i\rangle$ and the Lanczos coefficients for the Hamiltonian. From the Lanczos coefficients we can calculate the final energies $E_{\mu}$ and the unitary matrix that performs the diagonalization $Q$. 
4 Benchmark Calculations of Electromagnetic Sum Rules

4.1 Introduction

Electromagnetic transitions in atomic nuclei can reveal important information about the dynamical structure of the nucleus. The response function for a given nucleus and energy characterizes these transitions between an initial state, typically the ground state, and excited states. The energy moments of the response function are called sum rules. These sum rules are essential to calculating, e.g., the electric dipole polarizability of a nucleus [43] and nuclear polarization effects for muonic atoms [47]. Response functions and sum rules have been successfully calculated in the shell model [48] or using ab initio methods, such as hyperspherical harmonics (HH) and no-core shell model (NCSM) for light nuclei [36, 49, 50] or the coupled-cluster (CC) method for closed-shell nuclei [51–53]. The purpose of this work is to utilize the symmetry-adapted no-core shell model (SA-NCSM) [34, 35, 54] with the view toward first-principle applications to sum rules for open-shell nuclei up through the medium-mass region.

Recent work has illustrated that the reach of ab initio methods can now extend into the intermediate- and medium-mass region, both in terms of structure observables (e.g., see Refs. [34, 55–57]) and reaction observables (e.g., see Refs. [44, 58–61]). Specifically, since the introduction of the IT-NCSM [27], which was able to examine $^{40}$Ca in a no-core shell model space, and the emergence of many-body techniques that scale slowly with particle number, e.g., CC theory [62, 63], the in-medium similarity renormalization group (IM-SRG) [64], and self-consistent Green’s function (SCGF) theory [65], much of the intermediate- and medium-mass region is now accessible to ab initio methods. Further, the demonstration that the CC method can examine the closed-shell $^{100}$Sn nucleus [57] suggests that ab initio descriptions, albeit within some approximations, are feasible in heavy nuclei. This presents a unique opportunity for ab initio techniques to examine the robustness of available nuclear interactions and to study dynamical observables in this heavier mass region. To this end, the SA-NCSM has been shown to be a valuable approach capable of using only the physically-
relevant subspaces of the standard NCSM model space, thereby extending the reach of the NCSM toward heavier nuclei while maintaining important physical features, such as collectivity.

In this chapter, we present sum rules using the Lanczos sum rule method [46], where wave functions are calculated in the SA-NCSM many-body approach. The present results are reported for $^4$He, where exact solutions exist in the HH method and allow for a benchmark study for the same nucleon-nucleon (NN) interaction used in both methods. In particular, various electromagnetic sum rules are calculated for $^4$He in the SA-NCSM using the JISP16 [20], N3LO-EM [22], and NNLO$_{opt}$ [23] interactions. This includes non-energy weighted (NEWSR), energy weighted (EWSR), and inverse energy weighted sum rules for electric monopole ($L = 0$), dipole ($L = 1$), and quadrupole ($L = 2$) transitions. The results are benchmarked against the HH method and the standard no-core shell model (NCSM) [6, 66], and are found to agree with both methods within the uncertainties of the many-body techniques. In addition, for the N3LO-EM interaction, the role of the three-nucleon forces (3NF’s) is discussed in comparison to HH calculations with or without the 3NF’s. We also discuss techniques for handling spurious center-of-mass (CM) excitations in many-body methods that use laboratory-frame coordinates. Specifically, we detail a novel use of the Lawson procedure to calculate SA-NCSM sum rules, where the CM spurious can be removed exactly. Further, we show that the SA-NCSM can be applied in the Lorentz integral transform method (LIT), which, in turn, can be used to calculate translationally-invariant response functions for intermediate- and medium-mass nuclei.

4.2 Theoretical framework

4.2.1 Symmetry-adapted no-core shell model (SA-NCSM)

The SA-NCSM framework [34] is an *ab initio* no-core shell-model approach with a symmetry-adapted basis. In this work, we use an SU(3)-coupled basis. We employ the many-body $N_{\text{max}}$ truncation where we enumerate all many-body states, with the selected symmetries, possessing total harmonic oscillator (HO) excitation quanta less than or equal to
Specifically, the $N_{\text{max}}$ cutoff is defined as the maximum number of HO quanta allowed in a many-particle state above the minimum for a given nucleus. Hence, basis states where one nucleon carries all the $N_{\text{max}}$ quanta are included, in which cases one nucleon occupies the highest HO shell.

The SA-NCSM allows one to down-select from all possible configurations to a subset that tracks with an inherent preference of a system towards low-spin and high-deformation dominance – and symplectic multiples thereof in high-$N_{\text{max}}$ spaces [35] – as revealed to be important in realistic NCSM wave functions [67,68].

The many-nucleon basis states of the SA-NCSM are decomposed into spatial and intrinsic spin parts, where the spatial part is further classified according to the SU(3)$\supset$SO(3) group chain. The significance of the SU(3) group for a microscopic description of the nuclear collective dynamics can be seen from the fact that it is the symmetry group of the successful Elliott model [11, 12], and a subgroup of the physically relevant Sp(3, $\mathbb{R}$) symplectic model [29, 30, 69], which provides a comprehensive theoretical foundation for understanding the dominant symmetries of nuclear collective motion. The SA-NCSM basis states are labeled schematically as

$$|\vec{\gamma}; N(\lambda \mu)\kappa L; (S_pS_n)S; JM\rangle,$$

where $S_p$, $S_n$, and $S$ denote proton, neutron, and total intrinsic spins, respectively. $N$ is the total number of HO excitation quanta. The values $(\lambda \mu)$ represent a set of quantum numbers that labels an SU(3) irreducible representation, or “irrep” – they bring forward important information about nuclear shapes and deformation, according to an established mapping [29, 70, 71]; for example, (00), $(\lambda 0)$ and $(0 \mu)$ describe spherical, prolate and oblate deformation, respectively. The label $\kappa$ distinguishes multiple occurrences of the same orbital momentum $L$ in the parent irrep $(\lambda \mu)$. The $L$ is coupled with $S$ to the total angular momentum $J$ and its projection $M$. The symbol $\vec{\gamma}$ schematically denotes the additional quantum numbers needed to specify a distribution of nucleons over the major HO shells and their single-shell and inter-shell quantum numbers.
Similarly to the NCSM, where $N_{\text{max}}$ is used to denote the model space, in the SA-NCSM, we adopt a notation where an SA-NCSM model space of “$(N_0)N_{\text{max}}$” includes all the basis states up through $N_0$ total excitation quanta and a selected set of basis states in $N_0 + 2, N_0 + 4, \ldots$ up through $N_{\text{max}}$. The selection is based on high-deformation and low-spin dominance, along with symplectic $\text{Sp}(3, \mathbb{R})$ excitations thereof. Hence, configurations of largest deformation (typically, large $\lambda$ and $\mu$) and lowest spin values are included first. This ensures that the SA-NCSM model spaces accommodate highly-deformed configurations with high-energy HO excitations together with essential mixing of low-energy excitations [35, 67, 68].

4.2.2 Hyperspherical harmonics (HH)

In the hyperspherical harmonics (HH) method and its effective interaction counterpart, the EIHH method [72–75], the $A$-body problem is solved using a basis of hyperspherical harmonics (HH), which are functions of $A - 1$ Jacobi vectors, where the center-of-mass has been removed. In this case, it is convenient to write the Jacobi vectors using hyperspherical coordinates, i.e., a hyperradius $\rho$ and $3A - 4$ hyperangles $\hat{\Omega}$. The intrinsic Hamiltonian in these coordinates is

$$\hat{H} = \frac{1}{2m} \left[-\Delta_{\rho} + \frac{\hat{K}^2}{\rho^2}\right] + V,$$  \hspace{1cm} (4.2)

where $V$ is the interaction, $\Delta_{\rho}$ acts only on $\rho$, and $\hat{K}^2$ is the hyperangular momentum operator. The HH are eigenfunctions of $\hat{K}^2$, parametrized by the hyperspherical quantum number $K$. In practice, the model space is truncated at some value $K_{\text{max}}$, and the problem is reduced to a parametrized one-dimensional integral equation on $\rho$, which is solved numerically as described in Refs. [72, 73, 75].

4.2.3 Lanczos sum rule (LSR) method

The response of a nucleus to external perturbation of energy $E_x$, e.g., electromagnetic perturbation, can be characterized using the corresponding response function
\[ R(E_x, E_i) = \sum_f |\langle \psi_f | \hat{O} | \psi_i \rangle|^2 \delta (E_f - E_i - E_x), \]  

(4.3)

associated with the operator \( \hat{O} \) that induces a transition from the initial state \( |\psi_i \rangle \) into a set of final states \( |\psi_f \rangle \). In contrast to the equations in Ch. 3, we have chosen to write the response function in terms of \( E_x \) and \( E_i \) to better emphasize its physical interpretation. Here, \( |\psi_{i(f)} \rangle \) and \( E_{i(f)} \) are eigenstates and the corresponding eigenvalues, respectively, of the Hamiltonian \( \hat{H} \), and \( \mathcal{F}_f \) includes the entire discrete and continuous spectrum, i.e., \( \mathcal{F}_f |\psi_f \rangle \langle \psi_f| = 1 \).

In this work, we focus on several moments of the response function, i.e., sum rules of the form

\[ m_n = \int dE_x R(E_x, E_i) E_x^n, \]  

(4.4)

which, using the completeness of the eigenstates \( |\psi_f \rangle \), can be rewritten as

\[ m_n = \langle \psi_i | \hat{O}^\dagger \left( \hat{H} - E_i \right)^n \hat{O} |\psi_i \rangle. \]  

(4.5)

This suggests that the calculation of \( m_n \) does not require explicit knowledge of the response function. Furthermore, if the transitional state \( \hat{O} |\psi_i \rangle \) is localized or well described within the range of the interaction, then it is justified to use a bound-state method to calculate the wave function \( |\psi_i \rangle \) and \( m_n \).

Of particular interest is the zeroth moment \( m_0 \) or the square of the norm of the transitional state \( \hat{O} |\psi_i \rangle \)

\[ m_0 = \langle \psi_i | \hat{O}^\dagger \hat{O} |\psi_i \rangle, \]  

(4.6)

which is also known as the non-energy weighted sum rule (NEWSR) or the total strength of the response, \( \int dE_x R(E_x, E_i) \). In this paper, we study sum rules \( m_0, m_1, \) and \( m_{-1} \) for \( |\psi_i \rangle \) being the ground state.

To calculate \( m_n \), we use the Lanczos sum rule (LSR) method (see, e.g., [45, 46] and references therein), which is especially suitable for computing the low-lying energy spectrum.
that contains the peaks of the electromagnetic transitions under considerations, that is, electric monopole, dipole, and quadrupole transitions. The LSR method solves for each sum rule using

\[ m_n = \langle \psi_i | \hat{O}^\dagger \hat{O} | \psi_i \rangle \sum_{k=0}^{N-1} |Q_{k0}|^2 (E_{x,k})^n, \]  

where \( N \) is the number of Lanczos iterations, \( Q_{k0} \) is the matrix that diagonalizes the tridiagonal matrix the Lanczos algorithm produces, and \( E_{x,k} \) is the excitation energy of the \( k \)-th state. The method benefits from a suitable choice of the Lanczos pivot, the starting point of the iterative tridiagonalization process. In particular, for the pivot, we use the normalized transitional state

\[ |\phi_0\rangle = \frac{\hat{O} | \psi_i \rangle}{\sqrt{m_0}}. \]  

The LSR method has been shown to be very efficacious \[46\] and has reached the required precision in the calculation of dynamical nuclear effects in the Lamb shift of light muonic atoms \[76\].

Alternative ways to calculate the dipole inverse-energy-weighted sum rule using bound-state methods, such as HH and coupled-cluster methods, have been explored in Ref. \[43\]. Specifically, sum rules and response functions can be obtained without explicitly solving for the final eigenstates, by utilizing an indirect method, the Lorentz integral transform (LIT) method \[41, 77\]. The LIT method has been well documented in the literature and used to obtain nuclear responses for electromagnetic and weak operators, as detailed in Ref. \[41\]. For completeness, we present here the so-called LIT equation

\[ \left( \hat{H} - z \right) |\psi\rangle = \hat{O} | \psi_i \rangle \]  

where \( z = E_i + \sigma + i\Gamma \), \( \sigma \) and \( \Gamma \) determine the peak and width of the Lorentzian kernel, and \( E_i \) and \( | \psi_i \rangle \) are the energy and wave function for the initial state to be solved for in.
the SA-NCSM. The LIT equation provides solutions for $|\psi\rangle$, which, in turn, computes the Lorentz integral transform

$$L = \langle \psi | \psi \rangle = \frac{\Gamma}{\pi} \int dE_x \frac{R(E_x, E_i)}{(E_x - \sigma)^2 + \Gamma^2}. \quad (4.10)$$

From here, one can use the Lanczos coefficients computed for Eq. (4.9) that uniquely determine $L$, as shown in Eq. (3.40) of Ref. [41].

4.2.4 Removal of the spurious center-of-mass for laboratory-frame calculations

The proper handling of the center-of-mass (CM) excitations is essential for methods that use laboratory-frame coordinates. A well-established method to remove CM spuriosity in the resulting energy spectrum is to use the Lawson procedure [10] that shifts states containing CM excitations to higher energies. This results in low-lying states in the energy region of interest that are translationally invariant.

A very important feature of the SA-NCSM is that any SA-NCSM selected model space permits exact factorization of the center-of-mass motion [9]. This feature is present in the NCSM, however, it does not hold for any selection of the NCSM model space. In the SA-NCSM, it remains valid only as a result of the SU(3) symmetry used for the selection. Hence, a selected model space yields eigenfunctions that exactly factorize into a product of center-of-mass and intrinsic components, $|\Psi_{cm}\rangle |\psi_{intrinsic}\rangle$. The Lawson procedure [10] uses a Lagrange multiplier term that is added to a Hamiltonian expressed in laboratory-frame coordinates, $\hat{H} + \lambda \hat{N}_{cm}$, where $\hat{N}_{cm}$ is the operator that counts the number of CM excitations and $n_{cm}$ is its eigenvalue. For a typical value of $\lambda \sim 50$ MeV, the nuclear states of interest (with energy $\lesssim 30$ MeV) have wave functions that are free of center-of-mass excitations ($n_{cm} = 0$), while CM-spurious states ($n_{cm} > 0$) lie much higher in energy.

However, extra care must be taken when calculating observables with these eigenvectors. The reason is that the eigenfunctions are not the intrinsic wave functions, but contain the
center-of-mass component with $n_{\text{cm}} = 0$. Hence, observables calculated with operators that are not translationally invariant can induce CM excitations that affect the results. A number of approaches can be used to address this, and we find two efficient ways: 1) using a CM-free pivot or transitional state $|\phi_0\rangle$ (4.8), and 2) working with a CM-spurious pivot. In both cases, to compute the Lanczos coefficients for calculating sum rules and LIT, a Lawson term is used, $\hat{H} + \lambda \hat{N}_{\text{cm}}$. Note that this step is in addition to the one that uses the Lawson procedure in the eigenvalue problem to compute the $|\psi_i\rangle$ initial state and that this state is always free of CM excitations.

1) **CM-free pivot.** – In general, a translationally-invariant transitional state $\hat{O}|\psi_i\rangle$ can be obtained for a translationally-invariant operator $\hat{O}$, for which the laboratory-frame coordinates $r_n$, $n = 1, 2, \ldots, A$, are replaced by $(r_n - R_{\text{cm}})$ for a center-of-mass coordinate $R_{\text{cm}} = \frac{1}{A} \sum_n r_n$. This, however, means that one needs to handle many-body operators instead of the original one-body electromagnetic operators. In our work, we adopt an alternative procedure, that is, we use a projection operator to project out the CM-free component of the transitional state. We use the projection operator

$$\hat{P} = \prod_{n_{\text{cm}}=1}^{N_{\text{max}}} \left( \mathbb{1} - \frac{\hat{N}_{\text{cm}}}{n_{\text{cm}}} \right). \quad (4.11)$$

This operator will project out only the states with $n_{\text{cm}} = 0$, thereby removing the contribution of the CM excitations up to $N_{\text{max}}$, the model-space cutoff for the $|\psi_i\rangle$ wave function. The norm can then be calculated, yielding a CM-free $m_0$ moment, which is, in turn, used to calculate the CM-free pivot via Eq. (4.8).

2) **CM-spurious pivot.** – An alternative approach is to use an operator $\hat{O}$ that is not translationally invariant to obtain a CM-spurious transitional state. The CM-spurious pivot is then calculated using Eq. (4.8), where the CM-spurious norm (or $m_0$) is used. We can then use the normalized pivot vector to initiate the Lanczos algorithm for a Hamiltonian that includes a Lawson term, $\lambda \hat{N}_{\text{cm}}$. This extra term will only act on CM-spurious states.
and thus shift all of them higher in the energy spectrum, as specified by the value of \( \lambda \). We can then use the Lanczos coefficients in either the LSR or LIT methods. A very important step here is that, for the LSR method, we need to select an energy cutoff to avoid including the higher-lying CM-spurious states, provided our choice of \( \lambda \) is large enough for a given moment \( m_n \) to converge (see Sec. 4.3.3 for illustrative examples). Similarly, for the LIT method we can consider an energy range that is appropriate to invert to find the response function, provided we have projected the CM contributions above that region.

### 4.3 Results and discussions

In this work, the aim is to illustrate the ability of the SA-NCSM to reliably calculate the necessary nuclear states required as input to sum rules with the LSR method and response functions with the LIT method. To achieve this, we study the convergence of results with increasing model spaces and compare the results to those obtained in the HH and NCSM models, as detailed in the following subsections. In particular, we discuss ground-state properties and sum rules for three operators: the electric (isoscalar) monopole, the electric (isovector) dipole, and the electric (isoscalar) quadrupole. These are respectively defined, in laboratory-frame coordinates, as

\[
\begin{align*}
\hat{M} &= \frac{1}{2} \sum_{i=1}^{A} r_i^2 \\
\hat{D} &= \sqrt{\frac{4\pi}{3}} \sum_{i=1}^{A} e_i r_i Y_{10}(\hat{r}_i) \\
\hat{Q} &= \sqrt{\frac{16\pi}{5}} \sum_{i=1}^{A} e_i r_i^2 Y_{20}(\hat{r}_i)
\end{align*}
\]

For all calculations, we use the well-established NN interactions JISP16 and N3LO-EM, and provide comparisons of the results obtained in the HH, NCSM, and SA-NCSM for each combination of interaction and operator. Note that NCSM and SA-NCSM calculations are only shown for \( h\Omega = 25 \text{ MeV} \) (unless otherwise indicated), while calculations were performed for a range of \( h\Omega \) values between 22 and 28 MeV to perform extrapolations to the infinite
model space and estimate model uncertainties. These extrapolations are based on the Shanks method [78,79] to determine the converged value of an infinite sum. In particular, one can use the Shanks transformation ansatz for a quantity $X_\infty = \sum_{n=0}^\infty x_n$ such that $X_N = \sum_{n=0}^N x_n$ is given by $X_N = X_\infty + AQ^N$ for large $N$, where $0 < Q < 1$. Typically, for data on a converging trend, it is sufficient to use the last three points to determine the infinite-space value,

$$X_\infty = \frac{X_{N_{\text{max}}+2}X_{N_{\text{max}}-2} - X^2_{N_{\text{max}}}}{X_{N_{\text{max}}+2} + X_{N_{\text{max}}-2} - 2X_{N_{\text{max}}}}$$  \hspace{1cm} (4.15)$$

where $X_\infty$ is the converged value of interest and $X_i$ is the unconverged value at different values of $N_{\text{max}}$. This calculation was performed for each value of $\hbar\Omega$ and those extrapolated values were used to estimate the combined theoretical uncertainty in each quantity. Note that these uncertainties are associated with convergence of the many-body SA-NCSM method, of relevance to the present benchmark study, and do not reflect uncertainties in the interaction used. In fact, for well-converged data, this procedure estimates model uncertainties much smaller than those anticipated from varying the interaction.

4.3.1 Nuclear observables and sum rules using the JISP16 NN interaction

The ground-state properties of $^4\text{He}$ are well converged in the HH, NCSM, and SA-NCSM methods and agree for all three methods, as shown in the plots of the ground-state energy and the point-proton rms radius as a function of the model-space size (Fig. 4.1). Note that we report on the ground-state properties because the non-energy weighted sum rule $(m_0)$ depends only on the structure of the operator and the ground-state wave function, in accordance with Eq. (4.6).

We also find good convergence with respect to $K_{\text{max}}$ or $N_{\text{max}}$ for all three methods in the sum rules, as shown in the plots of electric monopole, dipole, and quadrupole non-energy weighted sum rules, $m_0$ (Fig. 4.2).
Figure 4.1: Ground-state energy and point-proton rms radius for $^4$He as a function of $K_{\text{max}}$ or $N_{\text{max}}$. HH, NCSM, and SA-NCSM calculations are performed for the bare JISP16 NN interaction; NCSM and SA-NCSM points are shown for $\hbar \Omega = 25$ MeV, while the extrapolated values are based on a range of $N_{\text{max}}$ and $\hbar \Omega$ values. Uncertainties of the extrapolated values are smaller than the size of the plot markers.

A full comparison of non-energy weighted, energy weighted, and inverse energy weighted sum rules for JISP16 for all three methods used are shown on the left side of Table 4.1. There, we find good overall agreement between the HH results and the extrapolated values for NCSM and SA-NCSM results, either within the uncertainties or differing on the $\sim 1\%$ level. The extrapolated results are based on three values of $N_{\text{max}}$ ($N_{\text{max}} = 12, 14, \text{ and } 16$ for NCSM and $\langle 6 \rangle_{12}, \langle 6 \rangle_{14}, \text{ and } \langle 6 \rangle_{16}$ for SA-NCSM) and three values of $\hbar \Omega$ ($\hbar \Omega = 22.5, 25, 27.5$ MeV). Note the important inverse energy weighted sum rule for the dipole is well reproduced and constrained in both the NCSM and SA-NCSM approaches.
Figure 4.2: Non-energy weighted sum rule as a function of $N_{\text{max}}$ or $K_{\text{max}}$ for $^4$He: (a) total monopole strength ($L = 0$) and quadrupole strength ($L = 2$), along with (b) dipole strength ($L = 1$) and inset showing convergence of three $\hbar\Omega$ values toward the extrapolated infinite-space value. HH, NCSM, and SA-NCSM calculations are performed for the bare JISP16 NN interaction; NCSM and SA-NCSM points are shown for $\hbar\Omega = 25$ MeV, while the extrapolated values are based on a range of $N_{\text{max}}$ and $\hbar\Omega$ values. Uncertainties of the extrapolated values are smaller than the size of the plot markers.
Table 4.1: Non-energy weighted \( (m_0) \), energy weighted \( (m_1) \), and inverse energy weighted \( (m_{-1}) \) sum rules for monopole, dipole, and quadrupole transitions in \( ^4\text{He} \). HH, NCSM, and SA-NCSM calculations are performed for the bare JISP16, N3LO-EM, and N2LO_{opt} NN interactions; NCSM and SA-NCSM results are the extrapolated values and include estimated model uncertainties based on small variations in \( \hbar \Omega \). The uncertainties reflect convergence of the many-body method. See text for further discussion.

<table>
<thead>
<tr>
<th></th>
<th>JISP16</th>
<th>N3LO</th>
<th>N2LO_{opt}</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>HH</td>
<td>NCSM</td>
<td>SA-NCSM</td>
</tr>
<tr>
<td>Monopole ( L = 0 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( m_0 ) (fm^4)</td>
<td>22.68</td>
<td>22.74(1)</td>
<td>22.57(8)</td>
</tr>
<tr>
<td>( m_1 ) (fm^4MeV)</td>
<td>150.2</td>
<td>150.9(2)</td>
<td>150.6(3)</td>
</tr>
<tr>
<td>( m_{-1} ) (fm^4/MeV)</td>
<td>0.2502</td>
<td>0.2524(3)</td>
<td>0.240(5)</td>
</tr>
<tr>
<td>Dipole ( L = 1 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( m_0 ) (e^2fm^2)</td>
<td>0.8583</td>
<td>0.8581(1)</td>
<td>0.8566(7)</td>
</tr>
<tr>
<td>( m_1 ) (e^2fm^2MeV)</td>
<td>41.352</td>
<td>41.3123(3)</td>
<td>41.321(3)</td>
</tr>
<tr>
<td>( m_{-1} ) (e^2fm^2/MeV)</td>
<td>0.02279</td>
<td>0.022802(7)</td>
<td>0.02265(7)</td>
</tr>
<tr>
<td>Quadrupole ( L = 2 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( m_0 ) (e^2fm^4)</td>
<td>14.731</td>
<td>14.78(1)</td>
<td>14.62(6)</td>
</tr>
<tr>
<td>( m_1 ) (e^2fm^4MeV)</td>
<td>721.5</td>
<td>722.9(2)</td>
<td>723.86(8)</td>
</tr>
<tr>
<td>( m_{-1} ) (e^2fm^4/MeV)</td>
<td>0.3747</td>
<td>0.3763(4)</td>
<td>0.363(4)</td>
</tr>
</tbody>
</table>
Additionally, we show comparisons of the monopole and dipole energy weighted running sum for JISP16 in Fig. 4.3 as a function of excitation energy. While the detailed structure of these curves is slightly different – the NCSM and SA-NCSM curves both show more discrete jumps in the running sum, indicating isolated excited states with some transition strength to the ground state – it is important to note that the running sums converge to the same values for all three methods. Thus, while the fine details of the excitation spectrum is slightly different, all three methods are able to extract the same information about the sum rules regardless of basis.

![Figure 4.3](image)

Figure 4.3: Energy weighted sum rules for (a) monopole and (b) dipole transitions as a function of excitation energy for $^4$He. HH, NCSM, and SA-NCSM calculations are performed for the bare JISP16 NN interaction; HH results are shown for $K_{\text{max}} = 20$ whereas NCSM and SA-NCSM results are shown for $N_{\text{max}} = 16$ and $\langle 6 \rangle_{16}$, respectively, with $\hbar \Omega = 25 \text{ MeV}$.

### 4.3.2 Nuclear observables and sum rules using chiral potentials

Compared to JISP16, the ground-state properties of $^4$He with N3LO-EM are slower to converge for all three methods, as shown in Fig. 4.4a. The ground-state energy nears convergence, and achieves good agreement with the one calculated in the HH around $N_{\text{max}} = 16$. Nevertheless, as for JISP16, the extrapolated values for N3LO-EM agree remarkably well with the results of the HH within the estimated uncertainties.

To address the role of three-nucleon forces (3NF’s) in these sum rules, we have also
examined the dipole polarizability since it can be directly compared to experiment. The dipole polarizability $\alpha_D$ is defined as

$$\alpha_D = 2\alpha \int dE_x \frac{R(E_x, E_i)}{E_x} = 2\alpha \ m_{-1} \quad (4.16)$$

where $\alpha$ is the fine-structure constant and the inverse energy weighted sum rule $m_{-1}$ is evaluated for the dipole operator defined by Eq. (4.13). Previous work with realistic interactions has indicated that including 3NF’s reduces the value of $\alpha_D$ by as much as 15% [80]. As shown in Fig. 4.5, we find that by using realistic interactions designed to minimize the role of 3NF’s, e.g. NNLO$_{opt}$, we are able to bring our NN interaction results into close agreement with existing NN + 3NF results.

4.3.3 Center-of-mass considerations

To illustrate the use of the Lawson procedure discussed in Section 4.2.4, we show selected examples of sum rules for the use of 1) CM-free pivot and 2) CM-spurious pivot (Fig. 4.6). The effect of the Lawson term is clearly evident for the CM-spurious pivot, regardless of the interaction or the specific energy weighting. In particular, in the Lawson procedure, we can...
shift the CM-spurious states above a certain energy specified by the value of $\lambda$ we choose in the Lawson term, $\lambda N_{cm}$, as illustrated in Fig. 4.6. We can clearly resolve the contributions to the sum rules from the CM-spurious states that are shifted above the chosen $\lambda$ values of 50, 200, and 500 MeV. Given a large enough $\lambda$, the method can report a converged value for the sum rule, provided the convergence is reached at an energy less than $\lambda$. This feature can be found in both NCSM and SA-NCSM calculations. The values found from this technique agree well with those obtained in the HH, where calculations are performed in a Jacobi basis. They also reproduce the values obtained in the NCSM and SA-NCSM calculations when a CM-free pivot is used.

Furthermore, we find a similar feature in the LIT, as shown in Fig. 4.7. Again, there is clear evidence of the CM-spurious states, as they shift to higher energies when we increase $\lambda$. Since we must numerically invert the LIT to find the response function, we can use this procedure to shift the CM-spurious contribution above a given energy range and invert the LIT only below this energy range. As the LIT depends on the value of the translationally invariant $m_0$, the procedure to generate a CM-free LIT transform from a CM-spurious pivot requires two parts: calculate the CM-free $m_0$ as shown in Fig. 4.6, and then calculate the LIT curve using the CM-free $m_0$ and a value of $\lambda$ large enough to push the CM-spurious
Figure 4.6: (a) Quadrupole non-energy weighted sum rule from JISP16 in a \( \langle 6 \rangle_{16} \) model space and (b) dipole inverse square root energy weighted sum rule from N3LO in a \( \langle 7 \rangle_{17} \) model space for transitions in \(^4\text{He}\) as a function of excitation energy, calculated by using different values of the Lawson coefficient \( \lambda \).

states out of the energy range of interest to calculate the response function.

Figure 4.7: LIT with \( \Gamma = 10 \) MeV for quadrupole transitions in \(^4\text{He}\), calculated from the SA-NCSM in a \( \langle 6 \rangle_{16} \) model space with JISP16 and different values of the Lawson coefficient \( \lambda \).

4.4 Conclusions

We have presented ab initio results from the SA-NCSM model for various sum rules describing electric monopole, dipole, and quadrupole transitions in \(^4\text{He}\), and compared them to those obtained in the HH and NCSM methods. We used the JISP16 and N3LO interactions and showed that SA-NCSM calculations reproduce the corresponding HH and NCSM results either within the estimated many-body model uncertainties or within \( \sim 1\% \). This implies
that the SA-NCSM can be reliably used to calculate sum rules in light nuclei. The SA-
NCSM calculations can then be expanded to nuclei beyond the area of applicability for the
other \textit{ab initio} methods. We further detailed the use of a new Lawson procedure in the
NCSM and SA-NCSM methods to recover translationally invariant sum rules, which may
have applications in other many-body methods that use laboratory-frame coordinates. We
have found that one can use CM-spurious pivot in the Lanczos procedure, by ensuring that
a suitable Lawson term is used, that is, a term that shifts the CM-spurious states above
an energy cutoff where the sum rules have reached convergence. The sum rules are then
reported at this energy cutoff. Similarly, in the LIT method, which can be used to produce
response functions from these \textit{ab initio} methods, a suitable choice for the Lawson term can
shift the CM-spurious contribution to energies higher than the region used to invert the
LIT transform. In particular, this latter application may allow us to examine the underlying
dynamics of \textit{ab initio} response functions for open-shell intermediate- and medium-mass nuclei
accessible by the SA-NCSM.
5 Electromagnetic Response Functions

5.1 Introduction

Collective modes, such as giant resonances, are often readily identifiable in the response function. In general, they are broad resonances that exhaust a major portion of the corresponding sum rule [37]. These have long been studied via the random phase approximation (RPA), primarily through the use of schematic or phenomenological interactions [84, 85]. While some \textit{ab initio} methods are being used to study giant resonances in this way [51, 60], continued study via first principles can help elucidate both the underlying physics and the adequacy of our realistic interactions. Further, certain giant resonances have connections to other branches of physics, such as the giant monopole resonance and its connection to the compressibility of nuclear matter. Nuclear compressibility is one of the main ingredients to the nuclear equation of state and its astrophysical applications span from core-collapse supernovae to neutron stars [86]. Thus, knowing the value of the compressibility precisely can help in performing these simulations.

5.2 Methods

5.2.1 Response functions

To calculate response functions, we continue to employ the symmetry-adapted no-core shell model (SA-NCSM) and the Lorentz integral transform (LIT) methods discussed in previous chapters. The SA-NCSM provides us with high-quality wave functions, which can be decomposed and examined in terms of individual basis states and their associated deformation. The LIT method allows us to calculate response functions directly from these SA-NCSM wave functions and knowledge of the operator describing the transitions we are examining. Here, we do not perform the inversion of the LIT to retrieve the response function, but instead take the limit of small width $\Gamma$ to recover a discretized response folded with a Lorentzian. This approach is sometimes called the Lanczos response method [41, 87] and it allows us to study properties of the excited states, including fragmentation of giant resonances, without having to worry about the delicate inversion process required by the
5.2.2 Nuclear compressibility

With the ability to calculate response functions and examine giant resonances, another natural application of this approach would be to investigate giant monopole resonances and their connection to nuclear compressibility. The second-order derivative of the binding energy per particle gives us information about the stiffness of nuclear matter against variations in the density [37]. This defines a compression modulus for infinite nuclear matter

\[ K_\infty = k_F^2 \frac{d^2}{dk_F^2} \left( \frac{E}{A} \right)_{k_F=k_{F0}}, \quad (5.1) \]

where \( k_F \) is the Fermi momentum.

Previous work has shown that we can write the compressibility of a finite nucleus \( K_A \) as

\[ K_A = K_{\text{vol}} + K_{\text{surf}} A^{-1/3} + K_{\text{Coul}} Z^2 A^{-4/3} + K_{\text{sym}} \left( \frac{N - Z}{A} \right)^2, \quad (5.2) \]

where \( K_{\text{vol}}, K_{\text{surf}}, K_{\text{Coul}}, K_{\text{sym}} \) are the volume, surface, Coulomb, and symmetry contributions to the compressibility of an \( A \)-body system and \( N \) (\( Z \)) is the neutron (proton) number [88]. In order to determine these coefficients, it is tempting to relate this expression for \( K_A \) to the semi-empirical mass formula [89], however such approaches have been shown to be unreliable in previous work. As such, usually one connects \( K_A \) to the energy of the giant monopole resonance (GMR) via

\[ K_A = \frac{m}{k^2} \langle r^2 \rangle E_{\text{GMR}}^2, \quad (5.3) \]

where \( m \) is the mass of the nucleon and \( \langle r^2 \rangle \) is the rms matter radius [88]. In the so-called macroscopic approach, one would find \( K_A \) values for a variety of nuclei from Eq. (5.3) and then use that data to fit the coefficients in Eq. (5.2). In principle, \( K_{\text{vol}} \) can then be
connected to $K_{\infty}$ [90,91]. Previous work has shown this works fairly well, but the values of $K_{\infty}$ it produces can have fairly large uncertainties [37].

The other popular approach is called the microscopic approach [91]. It starts with a microscopic nuclear interaction and typically utilizes an approach based on the Hartree-Fock method that calculates the binding energy per nucleon as a function of the Fermi momentum [92]. Recently, chiral potentials have been employed (e.g., see Ref. [93]).

In our approach, we take advantage of the SA-NCSM capability to provide accurate sum rules, where

$$E_{\text{GMR}} = \sqrt{\frac{m_1}{m_2}},$$  \hspace{1cm} (5.4)

An estimate for $K_A$ can be then given by Eq. (5.3).

Other approaches tend to combine some portion of the macroscopic and microscopic approaches in an attempt to reduce the amount of information one needs to calculate $K_{\infty}$, while also maintaining reasonable estimates for the uncertainty [86].

5.3 Results and discussions

5.3.1 $^4$He

Continuing from Ch. 4, we will first examine the $^4$He response functions calculated from the Lanczos response method. In this approach, we can see that the NCSM and SA-NCSM response functions are in good agreement, regardless of the operator (Fig. 5.1). This implies that we can expect our SA-NCSM response functions to be reliable for heavier nuclei, even in model spaces beyond the reach of the standard NCSM. For later applications to $K_{\infty}$, we report a centroid energy for the monopole distribution in $^4$He as 27.0(1) MeV.

5.3.2 $^{16}$O

Examining the monopole response for $^{16}$O (Fig. 5.2), we see one well-defined peak in the response function around 23.5 MeV. Using the ability of the SA-NCSM to examine the
Intrinsic deformation of the states contributing to this peak, we see strong evidence of the giant monopole resonance. Specifically, this peak is dominated (> 60%) by a (2 0) state of correlated $2\hbar\Omega$ one-particle excitations, which is inline with expectations we would have when comparing to previous work from symplectic shell models and analytic interactions. Here, we see this emerging from the realistic interaction $\text{NNLO}_{\text{opt}}$.

Figure 5.1: (a) Monopole, (b) dipole, and (c) quadrupole response functions for $^4\text{He}$ from the NCSM and SA-NCSM with $\text{NNLO}_{\text{opt}}$ in $N_{\max} = 14$ and $N_{\max} = \langle 6 \rangle 14$ model spaces, respectively. All of the response functions are shown for a width of $\Gamma = 4$ MeV and $\hbar\Omega = 25$ MeV.

If we apply Eq. (5.4), and use small variations in $\hbar\Omega$ to estimate an uncertainty, we find a centroid energy of 24(1) MeV. Experimental work on the giant resonances in $^{16}\text{O}$ have found values consistent with this range, e.g. Ref. [94] and references therein.

Figure 5.2: The monopole response function for $^{16}\text{O}$ in a $\langle 2 \rangle 10$ model space, calculated with $\text{NNLO}_{\text{opt}}$, $\hbar\Omega = 16$ MeV, and a width of $\Gamma = 2$ MeV.
5.3.3 $^{20}$Ne

Moving toward an open-shell nucleus, the monopole response for $^{20}$Ne is shown in Fig. 5.3. Unlike the $^{16}$O case, the GMR strength is no longer concentrated in a single peak, but is instead fragmented across the energy range $20 - 40$ MeV. The largest contributions to these peaks still show evidence of the giant resonance. In particular, the first peak $\sim 20$ MeV contains $2\hbar\Omega$ excitations of the $(8\ 0)$ configuration that is known to dominate the ground state. Similarly, the peak $\sim 40$ MeV is dominated (> 40%) by a different $2\hbar\Omega$ excitation of the $(8\ 0)$ ground state configuration.

![Figure 5.3](image)

Figure 5.3: The monopole response function for $^{20}$Ne in a $\langle 2 \rangle_{10}$ model space, calculated with NNLO$_{opt}$, $\hbar\Omega = 15$ MeV, and a width of $\Gamma = 2$ MeV.

While not as concentrated as the $^{16}$O distribution, we can still estimate a centroid for the $^{20}$Ne GMR using Eq. (5.4). With small variations in $\hbar\Omega$, we find a centroid energy of $25(1)$ MeV.

5.3.4 Nuclear compressibility

With the reported centroid energies for $^4$He, $^{16}$O, and $^{20}$Ne, we can use Eq. (5.3) to calculate $K_A$, the compressibility of these $A$-body systems. These results are shown in Fig. 5.4 and are used, as a proof-of-principle study, to provide an estimate for the infinite matter compressibility. Without solely relying on either the macroscopic or microscopic approach, we can instead combine them and take these three data points and fit to Eq. (5.2).
As all of the data points involve symmetric nuclei \((N = Z)\), the symmetry term will vanish. This fit yields a compressibility for infinite nuclear matter of \(K_\infty = 185(5)\) MeV from the NNLO\textsubscript{opt} interaction, which is a reasonable estimate given the very limited set of nuclei under consideration. This value is below the generally accepted value \(250 < K_\infty < 315\) MeV [95], though this is expected. It has been known that NNLO\textsubscript{opt} cannot adequately describe infinite nuclear matter [96].

![Figure 5.4: The compressibility of an \(A\)-body system as a function of mass number. The black line is a fit to data.](image)

The approach described above represents a fully microscopic prescription to calculate \(K_\infty\). It does not require infinite nuclear matter calculations, nor does it require experimental data. With the addition of more nuclear data, this approach holds promise to reduce uncertainties in \(K_\infty\).

5.4 Conclusions

We have presented \textit{ab initio} response functions from the Lanczos response method, using SA-NCSM wave functions as input. These include response functions for \(^4\)He, \(^{16}\)O, and \(^{20}\)Ne, where the SA-NCSM wave functions were calculated using the NNLO\textsubscript{opt} NN interaction. The \(^4\)He SA-NCSM response functions were in good agreement with response functions calculated using the standard NCSM, regardless of whether we were examining the monopole, dipole, or quadrupole transitions. We used the \(^{16}\)O and \(^{20}\)Ne response functions to examine their respective giant monopole resonances and reported on the intrinsic deformation of
the underlying states contributing to the giant resonance peaks. We also provided a quick estimate for the compressibility of nuclear matter, as calculated from NNLO$_{opt}$, based on the GMR centroid energies $E_{GMR}$ and the compressibility of a finite nucleus $K_A$. Overall, these results indicate the SA-NCSM is well-positioned to calculate response functions for open-shell nuclei and to explore collective features of nuclei from first principles.
6 Conclusion

In this work we detailed an approach that combines results from the symmetry-adapted no-core shell model (SA-NCSM) with the Lorentz integral transform (LIT) method, the Lanczos sum rule (LSR) method, and the Lanczos response function method. Our goal was to assess the applicability of the SA-NCSM to calculations of dynamic quantities, such as the response function, and determine if our symmetry-informed framework could adequately capture the underlying physics.

To accomplish this, we implemented the LSR method, starting from SA-NCSM results, for electromagnetic monopole, dipole, and quadrupole sum rules in $^4$He, with a variety of energy weightings and nuclear interactions, and benchmarked our results with the hyperspherical harmonics approach. We were able to estimate uncertainties in our theoretical calculations by varying the parameters of our model space and found good agreement across all the sum rules we investigated. Further, by examining the electric dipole polarizability, we noted that the use of nuclear interactions designed to reduce the effect of three-nucleon forces can overcome deficiencies in the use of only NN interactions.

We also illustrated a novel use of projection techniques to remove spurious center-of-mass contributions from our sum rules, which may find applications in other many-body techniques that use laboratory-frame coordinates. Additionally, we illustrated the use of this same projection technique to remove these spurious center-of-mass contributions from the LIT, thereby allowing us access to the full LIT theoretical framework should we wish to use it to calculate response functions.

We also implemented the Lanczos response function method, which allows us to examine discretized responses and through the SA-NCSM, we investigated the contributions of individual basis states to the characteristic peaks in our response functions. This included descriptions of $^4$He, $^{16}$O, and $^{20}$Ne, where the open-shell nucleus $^{20}$Ne is considered beyond the reach of many other many-body methods. We examined these peaks for their giant resonance properties and discussed fragmentation of the giant resonance in $^{20}$Ne. By probing
the giant monopole resonances, we were able to connect these microscopic calculations to
the compressibility of nuclear matter and propose a straightforward method to calculate this
property for any given nuclear interaction.

Overall, our results indicate that the SA-NCSM is well-suited to provide inputs to calcu-
lations for response functions and in fact is uniquely positioned to examine the underlying
contributions to certain features of response functions. Additionally, the SA-NCSM’s ability
to reach nuclei in the $pf$ shell suggests it could be a valuable resource to anyone looking to
calculate response functions or sum rules across a wide range of nuclei.
References


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Vita

Robert Baker is a native of Williamsport, Tennessee. He earned a bachelor’s degree from Austin Peay State University, majoring in physics and minoring in chemistry and mathematics. Always a fan of using high performance computing to solve problems, he decided to pursue a doctorate in theoretical nuclear physics at LSU in the fall of 2013.