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Alpha Capture Reaction Rates for Nucleosynthesis Within an Ab Initio Framework

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in

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by

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Abstract

Clustering in nuclear systems has broad impacts on all phases of stellar burning, and plays a significant role in our understanding of nucleosynthesis, or how and where nuclei are produced in the universe. The role of α particles in particular is extremely important for nuclear astrophysics: $^4\text{He}$ was one of the earliest elements produced in the Big Bang, it is one of the most abundant elements in the universe, and helium burning – in particular, the triple-α process – is one of the most important “engines” in stars. To better understand nucleosynthesis and stellar burning, then, it is important to develop theoretical frameworks that can describe clustering for exotic systems of interest, however, modeling nuclear systems with cluster substructures represents a major challenge for *ab initio* many-particle approaches.

This work presents a new framework for calculating alpha widths, asymptotic normalization coefficients (ANCs), and α-capture reaction rates for narrow resonances, using *ab initio* wave functions. The method considers the overlap between cluster configurations and shell-model states computed within a symmetry-informed no-core shell model framework, the no-core symplectic shell model and the *ab initio* symmetry-adapted no-core shell model. We validate the theory in the well-studied, highly-clustered $^{20}\text{Ne}$ system. In particular, we calculate the spectroscopic amplitude and alpha partial width for the low-lying excited $1^-$ state at 5.79 MeV in $^{20}\text{Ne}$, which is the resonance that dominates the alpha capture reaction rate for $\alpha + ^{16}\text{O}$ at astrophysical temperatures. This framework is used to study spectroscopic amplitudes, alpha partial widths, bound-state wave functions, and ANC for $\alpha + ^8\text{Be} \rightarrow ^{12}\text{C}$, $\alpha + ^{12}\text{C} \rightarrow ^{16}\text{O}$, $\alpha + ^{15}\text{O} \rightarrow ^{19}\text{Ne}$, and $\alpha + ^{16}\text{O} \rightarrow ^{20}\text{Ne}$. We predict the reaction rate for $\alpha + ^{15}\text{O}$, which is used in a simulation of an X-ray burst to determine the impact on nuclear abundances produced.
1 Introduction

One question humans have a deep interest in is, “where does all of this come from?” In nuclear physics terms, this can be rephrased, “where, how, and when in the universe are nuclei produced?”

Our current understanding is that the Big Bang lead to the early production of lithium, and massive amounts of hydrogen and helium, the most abundant nuclei in the universe. Everything produced after the Big Bang, which includes additional hydrogen, helium, and lithium, as well as all heavier isotopes, is synthesized in hot stars and stellar events through nuclear reaction processes. The production of nuclei in the universe is called nucleosynthesis.

There are a number of processes involved in nucleosynthesis, such as the Carbon-Nitrogen-Oxygen cycle (or CNO cycle), rapid neutron capture process ($r$ process), the slow neutron capture process ($s$ process), the rapid proton capture process ($rp$ process), and others. However, there remain many open questions about these processes that produce heavier isotopes. For example, we do not have definitive answers about where these processes take place. It was only very recently, with the 2017 multi-messenger observation of a neutron star merger, that we were able to observe evidence that $r$ process nuclei are produced in neutron star merger events [1]. The broader goals of nuclear astrophysics, then, are to help characterize nuclear processes involved in stellar burning, to inform our understanding of the stellar life cycle, and to explain the production of nuclei in the universe.

In order to address these open questions, broad collaborations have developed that draw input from nuclear theory and experiment, astrophysics observations, and theoretical astrophysics tools. These collaborations make use of multi-physics codes, such as the Modules for Experiments in Stellar Astrophysics (MESA) [2–6] and the KEPLER code [7] to model complex astrophysical environments.

Astrophysical models such as these need precise masses for hundreds of nuclei – many of which are highly unstable – as well as precise determinations of all of the relevant reaction rates involving those nuclei. Typically, these rates are taken from nuclear reaction databases,
such as Nuclear Astrophysics Compilation of REactions (NACRE) [8] and the Joint Institute for Nuclear Astrophysics (JINA) Reaclib Database [9]. These databases contain experimentally measured data and data that is extracted from experiment through model-dependent methods. In addition, databases consist of evaluations, where known data are essentially extrapolated to provide estimates for reaction rates in systems that cannot or have not been measured. Although these extrapolations are based on good physics, and done using high-quality data, they can sometimes be very different from the true reaction rates in these systems. An illustrative, albeit extreme example of how reaction rates predicted through nuclear evaluations can differ from measured rates is given in Ref. [10], where the measured thermal neutron capture cross section of $^{88}$Zr was found to be five orders of magnitude larger than data evaluations predicted.

One role of nuclear physics in these interdisciplinary collaborations, then, is to identify unmeasured or otherwise unknown reactions to which simulations are highly sensitive, and to provide data for these systems in order to better constrain the nuclear physics component of the multiphysics simulations. Nuclear theory can help to meet these goals by providing reaction data for systems that are difficult or expensive to measure experimentally, especially systems near the driplines, which tend to be very short-lived and are expected to have low-lying isolated resonances. Additionally, nuclear theory can be used to characterize clustering phenomena in nuclei, which is instrumental in understanding nuclear reactions for astrophysics [11].

Nuclear reaction theory has historically been dominated by few-body methods, which identify important cluster substructures involved in a nuclear reaction, and treat those clusters in some kind of mean field approach. Specifically, Hauser-Feshbach codes such as EMPIRE [12], TALYS [13], and CCONE [14] have been relied on for describing compound reaction mechanisms, while optical model potentials (OMP) within a distorted wave Born approximation (DWBA) framework (see: Fresco code [15, 16]), have been used to describe direct reactions.
There has been a push in recent years toward more ab initio techniques, from OMPs derived from ab initio wave functions [17–20], to even a fully ab initio many-body no-core shell model with continuum (NCSMC) [21] approach for very light systems, to ab initio calculations of alpha-alpha scattering using lattice Monte Carlo simulations [22]. The present work aims to contribute to this effort by presenting a new method for calculating alpha widths and alpha-capture reaction rates through narrow resonances in nuclei below the calcium region. Using ab initio wave functions as input, we test the theory in $^{20}\text{Ne}$, and provide alpha-capture reaction data computed for nuclei of mass $A = 6 − 19$.

Chapter 2 discusses the context in which these reaction rates are used in astrophysics, gives more detail about multi-physics codes for astrophysics and the role of nuclear reaction rates in simulations, and motivates the need for a tool for determining alpha-capture reaction rates within the context of nuclear astrophysics. In Chapter 3, we will discuss the symmetries that emerge naturally from first-principles nuclear structure calculations, and the models that employ these symmetries to compute nuclear wave functions. Specifically, this chapter motivates the use of the symplectic symmetry through an introduction to the no-core symplectic shell model (NCSpM), which was applied by the author and collaborators to the structure of $^{12}\text{C}$, including a description of the highly-clustered Hoyle state. Chapter 4 will give the general background needed for understanding nuclear reactions from a few-body perspective, including defining important observable quantities in nuclear reactions, and how those observables are measured or calculated. The theory that underpins the results for this dissertation is presented in Chapter 5, which gives the derivation of a new many-body reaction theory, and provides a validation of the theory for the $^{16}\text{O}(\alpha, \gamma)^{20}\text{Ne}$ alpha capture reaction. Finally, Chapter 6 provides further application of the theory outlined in Chapter 5 in a broad study of astrophysically important nuclei, including another look at the Hoyle state in $^{12}\text{C}$.
2 Nuclear Astrophysics Motivation

The goals of nuclear astrophysics are to help characterize nuclear processes involved in stellar burning, to inform our understanding the stellar life cycle, and to explain the production of nuclei in the universe. This chapter gives a brief discussion of X-ray bursts, with a focus on the nuclear physics processes involved, and how this can inform our understanding of nucleosynthesis. We will discuss the relationship between observational data and astrophysical models, and how models depend on high-quality nuclear data. Section 2.2 motivates the importance of clustering for understanding both nuclear structure and reactions, and especially the importance of clusters for describing systems of importance in astrophysics. The final two sections of the chapter comprise a short review of the study of clustering in nuclear physics from both an experimental perspective (section 2.3) and a theoretical one (section 2.4), both of which lean heavily on reviews by M. Wiescher and T. Ahn [11], and Freer et al. [23].

2.1 X-ray Bursters

X-ray bursters (XRBs) are binary systems that typically consist of a main sequence star orbiting about an accreting neutron star. They are characterized by their repeated rapid increases in X-ray luminosity. There are two categorizations of XRBs, type-I and type-II, which differ in the underlying processes that drive the observed increase in X-ray flux. Here, we discuss only type-I XRBs. Type-I XRBs are the result of an unstable and explosive burning process – referred to as *thermonuclear runaway* – that takes place on the surface of the neutron star, and involves material accreted from the main sequence donor star. These explosive burning processes can persist for on the order of 10-100 s and are not cataclysmic, which allows for recurring bursts every few hours to days, and sometimes with an irregular pattern. An example of a regularly recurring Type-I XRB light curve is shown in Fig. 2.1.

These X-ray intensity profiles and the nuclear burning processes that drive them are not yet well understood: intensity profiles vary greatly in shape, duration, and burst frequency. Fig. (2.2) shows just one burst occurrence for three different observed XRBs, as a represen-
Figure 2.1: Figure taken directly from Ref. [24]. Light curve for the 4U/MXB 1820-30 system, shown over a 21 hour time period, showing seven bursts.

tative sample of just how different XRB light curves can be. Note that these bursts vary greatly: some are very short-lived, some take much longer to decay back to quiescence, and some have substructures within the burst peak [see the bottom right panel of Fig. (2.2)].

There are four important burning regimes that either drive energy production, or contribute to the short-lived high X-ray flux that characterizes the burst: (1) a hot CNO cycle, (2) the triple-$\alpha$ reaction, (3) the $\alpha$-$p$ process, and (4) the $rp$ process. The hot CNO I cycle comprises the quiescent burning regime, whenever a burst is not actively occurring. This CNO cycle heats up the system until the triple-$\alpha$ process is unlocked, along with two breakout reactions: $^{14}\text{O}(\alpha,p)^{17}\text{F}$ and $^{15}\text{O}(\alpha,\gamma)^{19}\text{Ne}$. The triple-$\alpha$ process is the main energy production mechanism through the rest of the burst sequence. The $^{14}\text{O}(\alpha,p)^{17}\text{F}$ leads to a second CNO bi-cycle (the hot CNO II cycle) [26], with its own breakout through the $^{18}\text{Ne}(\alpha,p)^{21}\text{Na}$ reaction. Once the system has reached energies high enough to break from the CNO I & II cycles (see Fig. 2.3), the flow is dominated by the $\alpha$-$p$ process: a series of $(\alpha,p)$ reactions on the $^{18}\text{Ne}$, $^{21}\text{Mg}$, $^{22}\text{Mg}$, $^{24}\text{Si}$, $^{25}\text{Si}$, $^{26}\text{Si}$, $^{30}\text{S}$, and $^{34}\text{Ar}$ isotopes [26,27]. This process is what drives the initial phase of thermonuclear runaway, which is observed as the XRB. The burst is also driven at slightly later times by the $rp$ process, which is a series of rapid proton captures that produces much higher-mass isotopes, up until it reaches a closed
Figure 2.2: Figure taken directly from Ref. [25]. X-ray intensities as a function of time observed by the Rossi X-ray Timing Explorer mission for XRBs: GS 1826-24 (top), 4U 1728-34 (bottom left), and 4U 2129+12 (bottom right). Each XRB light curve shows only one burst occurrence.

SnSbTe cycle [28]. Essentially all of the material accreted by the neutron star is consumed during the burst, and isotopes produced through these burning processes are retained on the surface of the neutron star because of its high gravity. This leftover material is often referred to as the ash from previous bursts, and its composition can have major impacts on the bursts that follow.

Because the X-ray intensity of the system is closely related to these underlying nuclear processes and to the ash from previous bursts, some significant work has been done to determine how sensitive modeled abundance patterns (which quantify ash production of a single burst) and light curves are to reaction rates involved in the burning.

2.1.1 Sensitivity Studies

Multi-physics codes, such as MESA [2–6] and Kepler [7] are used to model XRBs and produce theoretical abundance patterns and light curves. These codes account for the hydro-
dynamics of the system, mass transfer in binary systems, energy production through nuclear burning processes, and energy transfer through the environment, among other physics.

The nuclear physics in these models is characterized by the user through two main components: a list of all of the isotopes the user includes in their study (called the nuclear network), and a data file consisting of reaction rates needed to characterize burning. XRB nuclear networks can consist of anywhere from a few hundred [4,29] to over a thousand isotopes [30]. Reaction rates used in these models are typically taken from the JINA REACLIB database [9] or the NACRE database [8]. In sensitivity studies, reaction rates are typically increased and/or decreased one-by-one to determine their impact on XRB light curves and abundance patterns. For reactions that are not well-known or which are only known through data extrapolations, variations in the rate are often given by a fixed factor. For measured rates, variations are given by the uncertainty in the measured rate. Sample light curves produced in a Kepler-modelled XRB for an increased $^{15}\text{O}(\alpha,\gamma)^{19}\text{Ne}$, and a decreased rate are shown in Fig. 2.4. This reaction rate has been determined in multiple studies to have notable impact on XRB light curves, abundance patterns, and burst recurrence [9,29,31].
2.2 Alpha Clusters in Astrophysical Nucleosynthesis

Clustering in nuclei, and understanding nuclear systems through cluster models, is not new: Rutherford’s discovery of alpha radiation and his subsequent characterization of the alpha particle and alpha scattering [32–34], combined with the development of quantum mechanics began the era of studying nuclear clustering in earnest. In 1937, Wheeler developed the resonating group method (RGM) for describing clustering in nuclear systems [35,36], followed by a long series of other alpha cluster models for nuclear structure, and even including an effective $\alpha$-$\alpha$ scattering interaction [37–39]. When the notion that non-spherical collections of alpha particles, including linear chains, could be used to describe states in known $\alpha$-like nuclei (e.g., $^{12}$C, $^{16}$O, etc.) was proposed by Morinaga [40], it launched nuclear cluster physics into a decades-long focus on the Hoyle state in $^{12}$C and its impact on the triple alpha process [41]. The existence of cluster substructures in nuclei has a much broader impact
on astrophysics than the description of the Hoyle state, though: understanding clustering is imperative to accurately describe both quiescent and explosive stellar burning. There have been a number of reviews of clustering in nuclei [23, 42–49], but little direct work on understanding the impact of nuclear clusters in astrophysics, most of which is summed up in Ref. [11].

An alpha cluster is a substructure within a nucleus, wherein four nucleons that resemble a $^4\text{He}$ nucleus (i.e., two protons and two neutrons) are correlated such that they are, on average, much closer to one another than to the other particles in the system. In fact, this particular configuration of four nucleons is maximally correlated, so that nuclei composed of alpha particles (or \textit{alpha conjugate nuclei}), such as $^{12}\text{C}$, $^{16}\text{O}$, $^{20}\text{Ne}$, $^{24}\text{Mg}$, $^{28}\text{Si}$ etc., are more stable as a result of these high correlations. Because of this, alpha conjugate nuclei are significantly more abundant in the universe.

Cluster states in nuclei are simply states of the system that overlap strongly with a pure cluster configuration. Typically, cluster states occur near the threshold for dissociation into their expected cluster configuration [50], which is commonly illustrated using an Ikeda diagram (see Fig. 2.5). For example, the 7.65 MeV Hoyle state in $^{12}\text{C}$ is very near to the threshold for dissociation into three alpha particles at 7.27 MeV. Reactions of astrophysical importance typically take place through states near thresholds, where clusters dominate the structure of nuclei, and so the study of clustering in nuclei of great importance for astrophysics.

It is not only threshold states that exhibit clustering, however: evidence for clustering in the lowest-energy state of $^8\text{Be}$ [52] and the ground state of $^{16}\text{O}$ [53] have been seen, and cluster states may occur well below thresholds in neutron-rich nuclei [54]. These cluster structures can increase direct capture reaction cross sections (see Chapter 4 for more information about nuclear reactions and cross sections). So, understanding clustering in both resonant states near thresholds and in low-energy (and ground state) configurations is needed for determining reaction rates for nucleosynthesis.
2.3 Observing Cluster Structures in Nuclei

There are several important observables that relate to clustering in nuclei, but all observables fall into two categories: (1) observables related to deformation in the composite system, and (2) observables related to the reaction cross section. It should be noted that identifying large deformation in a system is not itself evidence of clustering: one can find highly deformed systems with very little clustering. However, cluster systems tend to be spatially extensive, which leads to enhanced $E2$ transition strengths and highly rotational features, as discussed below.

Highly deformed cluster states give rise to rotational bands. For sufficiently rotational systems, the moment of inertia can be deduced in a highly schematic way from the level spacing in a rotational band through the rotational model using $E_{rot} = J(J + 1)\hbar^2/2I$. For example, the rotational band built on top of the lowest $0^+$ state in $^8\text{Be}$ includes a 3.06
MeV $2^+$ state, and a $4^+$ state at 11.35 MeV. This is a highly rotational system: the ratio of the energies of the $4^+$ to $2^+$ states is 3.7, compared to the expected ratio for a purely rotational system of 3.33. For the $2^+$ state in $^8\text{Be}$, then, $\hbar^2/2I = 0.51$ MeV. Because of the proximity of the lowest $0^+$ state in $^8\text{Be}$ to the $\alpha + \alpha$ threshold, this highly rotational behavior can be associated schematically with two $\alpha$ particles separated by their touching distance (or twice the radius of the $\alpha$ particle) [23]. Cluster configurations involving larger clusters have asymmetric structures that give rise to parity doublet bands as have been seen in measurements of $^{13}\text{C}$ and $^{20,21}\text{Ne}$ [55,56].

Because of the high deformation of cluster states in nuclear systems, these states tend to also have large transition strengths. In particular, the high deformation of cluster states is associated with an extensive mean charge radius, which is directly related to the $E0$ transition operator. Measurements of these transitions are made in a number of ways: for example, the $^{11}\text{Be}(d,d')^{11}\text{Be}^*$ reaction exciting the $^{11}\text{Be}$ to the 8.65 MeV $3/2^+$ level was used to measure an $E0$ transition that was found to be quite large [57], and inelastic $\alpha$ scattering experiments on $^{16}\text{C}$ are used to identify prolate cluster states in that system [58–60]. In addition to the strong monopole transition strength, $E2$ transitions from one cluster state to another and their electric quadrupole moments are enhanced [11].

Finally, experimental cross sections and data extracted from those cross sections are some of the most important observables related to clustering. In particular, reduced cluster widths (especially $\alpha$ widths), spectroscopic factors, and transfer probabilities can indicate cluster structures. The width of a state is related through the uncertainty principle to the lifetime of the state: very short-lived states have a high probability to decay, and so have a large width. The total width of a state is determined by the sum of all partial widths, each of which is related to the probability for the state to decay by different means. Chapter 4 has a more lengthy discussion of partial widths in reaction theory.
The Wigner single-particle limit for the width $\Gamma_W$,

$$\Gamma_W = \frac{3\hbar^2}{2\mu r},$$

(2.1)

where $\mu$ is the reduced mass of the system, and $r$ is the separation between the clusters, gives an approximation for the width assuming a completely clustered system, similar to the schematic picture of $^8\text{Be}$ as two distinct but interacting $\alpha$ particles described above [61]. A width near the Wigner limit therefore indicates strong evidence of clustering. For example, the 1.5 MeV width of the $^8\text{Be} \, 2^+$ state is very close to the Wigner limit which supports the existence of a cluster substructure in this state [62]. Similarly, cluster states can be observed through inspection of the breakup probabilities, as in the study of the $^{12}\text{C} + ^{12}\text{C}$ cluster structure of $^{24}\text{Mg}$ through the $^{12}\text{C}(^{24}\text{Mg},^{12}\text{C}^{12}\text{C})^{12}\text{C}$ breakup reaction [63].

### 2.3.1 Direct and Indirect Measurements

Historically, cross sections have been determined by direct measurements of all contributing resonant and non-resonant processes to determine the resonance strength. This method is significantly hampered by the fact that reactions of astrophysical relevance occur at very low energies, below the Coulomb barrier, which greatly suppresses experimental yield and increases the error associated with background effects. This can be at least partially overcome through the use of deep underground experimental facilities that take advantage of natural shielding from the earth, such as the Laboratory for Underground Nuclear Physics (LUNA) accelerator facility in the Gran Sasso Laboratory in Italy. Additionally, some reactions involve such short-lived systems that direct measurements are simply not feasible. In these cases, it is sometimes possible to do studies in inverse kinematics, using stable targets and radioactive beams. The review paper [64] provides an excellent summary of ongoing efforts to improve inverse kinematics experiments with both stable and radioactive beams.

One can also measure differential cross sections through transfer and resonant scattering
reactions, which can be used to extract widths indirectly. The measured differential cross section is related in a model-dependent way to the spectroscopic factor ($SF$):

$$\frac{d\sigma_{\text{expt}}}{d\Omega} = (SF)N\sigma_{\text{DWBA}}$$  \hspace{1cm} (2.2)

where $N$ is the norm coefficient, and $\sigma_{\text{DWBA}}$ is the cross section predicted by a simple DWBA calculation. The reduced width $\gamma^2$ is directly related to the spectroscopic factor:

$$\gamma^2 = (SF)\gamma_W^2$$  \hspace{1cm} (2.3)

where $\gamma_W^2$ is the Wigner limit [61], and related to Eq. (2.1) as $\Gamma_W = 2P_l\gamma_W^2$, with penetrability denoted by $P_l$. There are more discussions of the partial with, reduced width, and penetrability in Chapter 5.

The near-threshold resonances that are important for astrophysics can also be probed using sub-Coulomb $\alpha$-transfer reactions to determine asymptotic normalization coefficients (ANCs). This method, called the ANC method, has been used in successful studies of the 5.79 MeV $1^-\text{ state in } ^{20}\text{Ne}$, using the $^{16}\text{O}(^{6}\text{Li},d)^{20}\text{Ne}$ transfer reaction and the bound $2^+$ and $1^-\text{ states of } ^{16}\text{O through the } ^{12}\text{C}(^{6}\text{Li},d)^{16}\text{O and } ^{12}\text{C}(^{7}\text{Li},t)^{16}\text{O transfer reactions} [65,66]$. The Trojan horse method (THM) is another indirect method in which a surrogate reaction is used to indirectly study the reaction of interest [67,68]. Generally, the THM would measure the reaction $A + (b + x) \rightarrow b + c + C$ to study the reaction $A + x \rightarrow c + C$. This method has been used to study a number of reactions, including $^2\text{H}(^{6}\text{Li},\alpha)^4\text{He}$, $^7\text{Li}(p,\alpha)^4\text{He}$, and $^{10}\text{B}(p,\alpha)^7\text{Be} [69]$. Because of the difficulty in measuring data – or extracting observables from measured data – for astrophysically relevant reactions, it becomes clear that theoretical approaches are necessary both in guiding experimental studies and in providing reaction data directly.
2.4 Clustering in Nuclear Models

Modeling nuclear systems exactly is complicated for two main reasons: (1) with increasing particle number, the number of degrees of freedom increases, (2) the nuclear interaction is not known exactly. This difficulty propagates into the study of clustering within nuclear systems: to describe clustering in an $A$-particle system exactly, one would need to solve an exact many-body method for the $A$-particle system for localized clusters that are spatially enhanced using a nuclear interaction derived from first principles, while taking care of antisymmetrization between the particles in the cluster states. The antisymmetrization, in particular, becomes computationally unfeasible for systems involving clusters with more than a few particles, or for systems involving more than three clusters. Later, we will discuss some promising results calculated within just such a framework. Typically, though, some combination of assumptions is made to simplify the problem.

Some early nuclear models made use of alpha particles as building blocks for modeling heavier systems, and therefore used effective interactions between alpha particles, rather than \textit{ab initio} nucleon-nucleon (\textit{NN}) interactions. These, we refer to as cluster models. There are also models that solve the many-body $A$-particle system, but which make use of effective interactions that enhance collective features. Finally, there are fully \textit{ab initio} models that treat particles independently and use realistic \textit{NN} interactions that are fit to the $pn$ and $pp$ scattering data. The following is a brief, and in no way exhaustive, outline of existing cluster models, many-body methods that make use of effective interactions, and \textit{ab initio} models.

2.4.1 Cluster Models

First studies of $\alpha$-$\alpha$ scattering were done within the framework of the resonating group method (RGM) \cite{35,36,70,71}, a microscopic cluster model. The RGM makes use of a cluster basis wave function for two clusters of $a$ and $A-a$ particles,

$$
\Psi = \mathcal{A}\{\psi_a\psi_{A-a}\chi(\xi)\},
$$

(2.4)
where $A$ is the antisymmetrizer, and must be applied to all nucleons comprising the cluster wave function. The clusters are described by their wave functions $\psi_a$ and $\psi_{A-a}$, respectively, and the relative motion $\chi(\xi)$ between the clusters is determined by solving the RGM equation, which is a Schrödinger-like equation. The RGM has great success in describing the relative motion between clusters, which easily lends itself to scattering problems, but is relegated to lighter systems; because the antisymmetrization increases in computational complexity with increasing $A$, the RGM becomes computationally cumbersome for heavier mass regimes.

The generator coordinate method (GCM) is another cluster model, but makes use of a basis of Bloch-Brink cluster wave functions. The Bloch-Brink cluster wave function is the antisymmetrized product of individual cluster wave functions $\psi_{C,S}$, each of which is localized to a particular region $S$ [72]. If all Bloch-Brink basis states needed to span the model space are included in the model, the GCM and RGM are equivalent [73]. However, the ability of the GCM to reduce the model space through including only the most important Bloch-Brink wave functions in the basis allows for the extension to heavier systems and systems involving multiple clusters. The extension of the GCM to nuclear scattering requires an extension of the basis to continuum states [74,75].

These microscopic cluster approaches have been used to study various reactions of astrophysical importance [75], and have been extended to apply to clustering in unstable systems, especially one- and two-neutron halo systems near the neutron drip line [76–79]. Results in these microscopic models compare reasonably with experimental data where it is available, and have made some predictions for the structure of highly exotic systems, such as $^{14}$Be [77]. In addition, the multi-channel GCM has been used to study the cluster structure of $^{12}$Be and $^{10}$Be [80–85].

Another cluster model that describes alpha conjugate nuclei in terms of a condensate of $\alpha$ particles, the Tohsaki-Horiuchi-Schuck-Röpke (TSHR) model, has been used to describe states in $^{12}$C and $^{16}$O, including the Hoyle state of $^{12}$C and the Hoyle-like $0^+$ state of $^{16}$O, as well as the ground state of $^{20}$Ne, as $\alpha$-cluster condensates [86,87].
The cluster basis used in the RGM has a complementary nature to the \( \text{Sp}(3, \mathbb{R}) \) symplectic group \([88,89]\), and a number of studies have taken advantage of that relationship. In particular, this approach has been used to describe alpha conjugate nuclei as binary cluster systems \([90–92]\), the sub-coulomb \( ^{12}\text{C} + ^{12}\text{C} \) resonances of \( ^{24}\text{Mg} \) \([93]\) of particular interest in astrophysics \([11]\), and overlaps between symplectic and cluster states for alpha conjugate nuclei \([94,95]\), which have been used to compute spectroscopic amplitudes \([96,97]\).

2.4.2 Many-Body Methods and \textit{Ab Initio} Approaches

There are a number of approaches to nuclear structure that do not assume clustering \textit{a priori}. The benefit of such approaches is that, although some use effective interactions, they can also use realistic \( \text{NN} \) interactions for a fully \textit{ab initio} description of clustering. Models such as the the Antisymmetrized Molecular Dynamics (AMD) method \([98–103]\) and the closely related Fermionic Molecular Dynamics (FMD) method \([104–108]\) and the no-core symplectic shell model (NCSpM) \([109,110]\) are many-body methods that do not assume clustering, but which typically use effective \( \text{NN} \) interactions. The FMD can be combined with the Unitary Correlation Operator Method (UCOM) to use effective interactions derived from realistic \( \text{NN} \) interactions \([108,111,112]\). Combining the AMD approach with self-consistent Hartree-Fock methods improves descriptions of valence neutron wavefunctions in halo nuclei, e.g., Beryllium isotopes \([113]\).

Because they do not assume alpha clustering \textit{a priori}, the AMD and FMD approaches have had great success in describing \( \alpha \)-cluster breaking in \( ^{12}\text{C} \) \([107,114–117]\) for improved low-energy spectra relative to pure cluster models. The AMD has also been used to describe the cluster substructure of the neutron-rich \( ^{22}\text{Ne} \) \([72]\). The NCSpM has been used to reproduce the low-lying spectrum of \( ^{12}\text{C} \) as well as collective and clustering features (see Chapter 3 and Refs. \([109,110]\)), and has been applied to a number of \textit{sd}-shell nuclei \([118,119]\).

The no-core shell model (NCSM) \([120,121]\) benefits from being a many-body method that can make use of both high-quality effective interactions as well as \textit{ab initio} interactions,
and has seen great success in providing nuclear structure data with quantified uncertainties. However, the \( m \)-scheme harmonic oscillator (HO) basis traditionally used within the NCSM is not sufficient for describing localized clusters, and is applicable to systems of about 12 particles. The symmetry-adapted no-core shell model (SA-NCSM) \cite{122} reorganizes the model space according to exact and dynamical symmetries of the spherical HO Hamiltonian associated with collective excitations. This allows for the extension to model spaces that include higher excitations needed to account for clustering. The model has thus far been applied strictly to the study of low-energy nuclear structure, including cluster substructures and \( E2 \) transitions in \( sd \)-shell nuclei from a fully \textit{ab initio} perspective \cite{123-127}.

The Green’s Function Monte Carlo (GFMC) method \cite{128} with a constrained path approximation has been used to describe the \( \alpha \)-cluster structure of \( 8 \)Be \cite{52} as well as the structure of the Hoyle state of \( 12 \)C and electromagnetic (EM) transitions to the \( gs \) \cite{129}. The Monte Carlo Shell Model \cite{130} has been used to study clustering, including two- and three-cluster formations in \( 6 \)He, \( 8 \)Be, and \( 10 \)Be \cite{131,132}.

Finally, nuclear lattice effective field theory (NLEFT) combines the chiral effective field theory (\( \chi \)EFT) \cite{133,134} with Monte Carlo techniques to solve the exact \( A \)-body problem. The Hoyle state was computed for the first time within an \textit{ab initio} framework using this method, albeit within a coarse lattice grid \cite{135}. The NLEFT has been used in conjunction with the adiabatic projection method (APM) \cite{136-140} to calculate the first \textit{ab initio} \( s \)- and \( d \)-wave phase shifts for the astrophysically relevant \( \alpha-\alpha \) scattering problem \cite{22}.

Hybrid approaches, which combine aspects of cluster models with \textit{ab initio} methods, take advantage of the best of both categories: (1) the predictive power that accompanies \textit{ab initio} methods, and (2) the ability to address scattering and reaction mechanisms through the inclusion of continuum effects. The no-core shell model with continuum (NCSMC) is one such approach. It extends the spherical HO basis of the NCSM with the continuum basis of RGM \cite{141,142}, and has been used to describe reactions involving single-particle and deuteron projectiles in two- and three-body reactions \cite{141-148}. A hybrid of the configuration
interaction technique and the RGM in a HO basis has been used to study cluster structures in $^{8,9}$Be, as well as the $3\alpha$ cluster structure of $^{12}$C [149].

A new microscopic method for determining the partial widths of resonances, and bound-state ANCs, for systems of astrophysical importance is described in this work. The following chapter outlines emergent symmetries in nuclear physics, the NCSpM, and the results of a study of the low-lying energy spectrum of $^{12}$C. It is followed by a discussion of the few-body perspective on nuclear reactions in Chapter 4.
3 Emergent Symmetries in Nuclear Physics

Symmetries have always played a significant role in theoretical approaches to nuclear structure and reactions. The 1963 Nobel prize in physics went to three nuclear physicists, two of whom – Maria Goeppert-Mayer, and J. Hans D. Jensen – shared half of it for their independent but concurrent development of the independent particle model, which is a microscopic model (meaning that it treats each particle in the system) built on the notion that nuclei can be described, to first order, by a spherical HO potential. Many modern nuclear structure models are built on exactly this framework, including the \textit{ab initio} NCSM [121,150] and its extensions (see Refs. [130,151,152]).

In the late 1950s, J. P. Elliott developed the SU(3) model, which attempted to bridge the gap between the independent-particle and collective pictures of nuclei [153,154]. Starting from a microscopic perspective, the SU(3) model describes deformation in nuclear systems through the use of the SU(3) symmetry. The Elliott SU(3) model has a multi-shell generalization in the symplectic shell model [155,156], which uses the \text{Sp}(3,\mathbb{R}) symmetry – an embedding group of SU(3) – in order to describe collective features of nuclei.

In this chapter, we will give some mathematical formalism for understanding the symplectic symmetry and its use in nuclear physics. We describe, here, a microscopic many-body nuclear structure model that makes use of a symplectic-preserving $NN$ interaction, and its application to the $^{12}\text{C}$ system. Of particular note is the ability of the model to reproduce the energy of the Hoyle state, and to begin probing collective features and clustering in $^{12}\text{C}$. The work presented in this chapter has been previously published by Dreyfuss \textit{et al.} [109,110].

3.1 The Symplectic Basis

The symplectic \text{Sp}(3,\mathbb{R}) symmetry applied in a microscopic framework is directly related to the particle position and momentum coordinates, and preserves rotations and vibrations of an equilibrium deformation [157,158]. Each irreducible representation (or \textit{irrep}) of the symplectic group can be thought of as a single shape, which is also allowed to rotate and vibrate. The equilibrium shape associated with a given irrep is called the \textit{bandhead}, and
associated excitations of this equilibrium shape are described through the application of the symplectic raising operator $A^{(2\sigma)}$. This operator introduces $2\hbar\Omega$ (see Fig. 3.1) 1-particle-1-hole (1p-1h) monopole or quadrupole excitations (one particle raised by two shells) together with a smaller $2\hbar\Omega$ 2p-2h correction for eliminating the spurious center-of-mass (CM) motion. The bandhead is the lowest-weight Sp(3,$\mathbb{R}$) state, which is defined by the requirement that the symplectic lowering operator $B^{(0\bar{2})} = (A^{(2\sigma)})^\dagger$ annihilate it. See Section 3.1.1 for more information about symplectic operators.

![Symplectic Irrep Diagram](image)

Figure 3.1: A schematic diagram of a symplectic irrep and its relationship to the HO, where HO shells are separated by $\hbar\Omega$ in energy. The bandhead of the illustrated symplectic irrep has $(\lambda_\sigma\mu_\sigma) = (8\,0)$. Excitations (de-excitations) are introduced through the symplectic raising (lowering) operator $A^{(2\sigma)} (B^{(0\bar{2})})$.

Each basis state in a symplectic Sp(3,$\mathbb{R}$) irrep is labelled according to the group chain [156],

$$
\text{Sp}(3,\mathbb{R}) \supset U(3) \supset SO(3) \supset SO(2), \quad (3.1)
$$

where $\sigma \equiv N_\sigma(\lambda_\sigma\mu_\sigma)$, and similarly, $n \equiv N_n(\lambda_n\mu_n)$, and $\omega \equiv N_\omega(\lambda_\omega\mu_\omega)$. The labels $(\lambda\mu)$
generally represent deformation, and are directly related to the more familiar $\beta$ and $\gamma$ shape parameters [159]. The label $\kappa$ tracks multiplicity in angular momentum $L$ for a given $\omega$, and $\rho$ tracks multiplicity of $\omega$ in the $\sigma \times n$ coupling. The total number of HO quanta associated with a particular symplectic state labelled in this way is given by $N_{\omega} = N_{\sigma} + N_{n}$.

A symplectic state is built through a symmetrically-coupled polynomial of symplectic raising operators acting on the bandhead as follows:

$$|\sigma \rho \omega \kappa LM\rangle = \left[ A^{(20)} \times \cdots \times A^{(20)} \right]^{(\lambda_{n} \mu_{n})} \times |N_{\sigma} (\lambda_{\sigma} \mu_{\sigma})\rangle^\rho_{\omega} .$$

$$N_{n}/2$$

The bandhead is an SU(3)-coupled many-body state with a given nucleon distribution over the HO shells; for a system of $A$ particles, the bandhead is associated with a set of \{\eta_1, \ldots, \eta_A\} configurations, where $\eta_i$ is the oscillator number associated with the $i$-th particle. The bandhead is labelled simply by the corresponding $N_{\sigma} \hbar \Omega$ energy of HO quanta\(^1\), together with the bandhead deformation, $(\lambda_{\sigma} \mu_{\sigma})$.

All of the states within a symplectic irrep share the same total spin $S_{\sigma}$, which is given by the spin of the bandhead $|\sigma; S_{\sigma}\rangle$. This spin dependence enters through the generalization

$$|\sigma \rho \omega \kappa (LS_{\sigma})JM_{J}\rangle = \sum_{MM_{S}} \langle LM; S_{\sigma} M_{S} |JM_{J}\rangle |\sigma \rho \omega \kappa LMS_{\sigma} M_{S}\rangle .$$

\(^1\)This includes the HO zero-point energy. To eliminate the spurious CM motion, we use $N_{\sigma}$, for which 3/2 is subtracted from the total HO quanta, together with symplectic generators constructed in relative coordinates with respect to the CM. These generators are used to build the basis, the interaction, the many-particle kinetic energy operator, as well as to evaluate observables.
ditional NCSM $M$-scheme basis (a basis of Slater determinants that have as a good quantum number the projection $M$ of the total angular momentum $J$) and the symplectic basis: if all possible $|\{\alpha\}\sigma\rangle$ irreps are included up to a given cutoff $N_{\text{max}}$ parameter, where $N_{\text{max}}$ indicates the HO excitations included in the model space above the ground state configuration, results calculated in an $M$-scheme basis truncated at that $N_{\text{max}}$ and a symplectic basis are the same for the same interactions.

### 3.1.1 Symplectic Operators in Nuclear Physics

The 21 intrinsic generators of the symplectic $\text{Sp}(3,\mathbb{R})$ group can be written in terms of the dimensionless HO raising and lowering operators, $b_{ja}^{(10)} = \frac{1}{\sqrt{2}}(r_{ja} - ip_{ja})$ and $b^{(01)}$ respectively, for each particle $j$ in an $A$-particle system. The position and momentum coordinates of the $j^{th}$ particle in the lab frame are $\vec{r}_j$ and $\vec{p}_j$, respectively, and $\alpha = 1, 2, 3$ enumerates the three spatial directions:

\[
A_{\mathcal{LM}}^{(20)} = \frac{1}{\sqrt{2}} \sum_{i=1}^{A} \{b_i^\dagger \times b_i\}_{\mathcal{LM}}^{(20)} - \frac{1}{\sqrt{2}A} \sum_{s,t=1}^{A} \{b_s^\dagger \times b_t\}_{\mathcal{LM}}^{(20)}
\]

\[
B_{\mathcal{LM}}^{(02)} = (-)^{\mathcal{L} - \mathcal{M}}(A_{\mathcal{LM}}^{(20)})^\dagger
\]

\[
C_{\mathcal{LM}}^{(11)} = \sqrt{2} \sum_{i=1}^{A} \{b_i^\dagger \times b_i\}_{\mathcal{LM}}^{(11)} - \sqrt{2} A \sum_{s,t=1}^{A} \{b_s^\dagger \times b_t\}_{\mathcal{LM}}^{(11)}
\]

\[
H_{00}^{(00)} = \sqrt{3} \sum_{i=1}^{A} \{b_i^\dagger \times b_i\}_{00}^{(00)} - \sqrt{3} A \sum_{s,t=1}^{A} \{b_s^\dagger \times b_t\}_{00}^{(00)}.
\]

There are six of the raising $A_{\mathcal{LM}}^{(20)}$ operators, six of the lowering $B_{\mathcal{LM}}^{(02)}$ operators (for both operators, $\mathcal{L} = \{0, 2\}$, with the normal projection $\mathcal{M} = \{-\mathcal{L}, -\mathcal{L} + 1, \ldots, \mathcal{L}\}$), eight $C_{\mathcal{LM}}^{(11)}$ operators ($\mathcal{L} = \{1, 2\}$), and one $H_{00}^{(00)}$ operator ($\mathcal{L} = 0$, only).

A number of operators of physical importance are $\text{Sp}(3,\mathbb{R})$-preserving, and can be con-
structured from the symplectic generators written above, including

\begin{align*}
\text{Angular momentum} & \quad L_{1M} = C_{1M}^{(11)}, \quad M = 0, \pm 1 \quad (3.8) \\
\text{Elliott quadrupole moment} & \quad Q_{2M}^{\text{Elliott}} = \sqrt{3} C_{2M}^{(11)} \quad (3.9) \\
\text{Mass quadrupole moment} & \quad Q_{2M} = \sqrt{3} \left( A_{2M}^{(20)} + B_{2M}^{(02)} + C_{2M}^{(11)} \right) \quad (3.10) \\
\text{Kinetic energy} & \quad \frac{T}{\hbar \Omega} = \frac{1}{\hbar \Omega} \sum_i \frac{p_i^2}{2m} \nonumber \\
& \quad = \frac{1}{2} H_{00}^{(00)} - \sqrt{\frac{3}{8}} \left( A_{00}^{(20)} + B_{00}^{(02)} \right) \quad (3.11) \\
\text{HO potential} & \quad \frac{V_{\text{HO}}}{\hbar \Omega} = \frac{1}{\hbar \Omega} \sum_i \frac{m \Omega^2 r_i^2}{2} \nonumber \\
& \quad = \frac{1}{2} H_{00}^{(00)} + \sqrt{\frac{3}{8}} \left( A_{00}^{(20)} + B_{00}^{(02)} \right) \quad (3.12)
\end{align*}

Because these important operators preserve the symplectic symmetry, they therefore act only within a single symplectic irrep. In other words, they do not mix symplectic irreps.

### 3.2 The No-Core Symplectic Shell Model

The NCSpM [110] takes advantage of the symplectic symmetry through the use of both a symplectic basis as well as a microscopic many-body $NN$ interaction with a single adjustable parameter. This model has been used to study $p$- and $sd$-shell nuclei [110,118], including $^{12}\text{C}$ and its elusive Hoyle State [109] without any parameter adjustment.

#### 3.2.1 A Schematic Many-Body Interaction

The Hamiltonian employed in this model consists of two components: (1) a single-particle term consisting of the familiar HO potential, as well as a spin-orbit term, and (2) a collective term which enters through the quadrupole-quadrupole interaction, tied to a long-range expansion of the $NN$ central force $V(|r_i - r_j|)$ [160]:

\begin{equation}
H_{\gamma} = \sum_{i=1}^{A} \left( \frac{p_i^2}{2m} + \frac{m \Omega^2 r_i^2}{2} - \kappa l_i \cdot s_i \right) + \frac{\chi}{2} \left( e^{-\gamma(Q \cdot Q - (Q \cdot Q)_N)} - 1 \right). \quad (3.13)
\end{equation}
This interaction has three parameters that are fixed using empirical estimates, \( \hbar \Omega \approx 41/A^{1/3} \), \( \kappa \approx 20/A^{2/3} \), (see, e.g., [161]) and \( \chi = \hbar \Omega / (4 \sqrt{N_\omega / N_\omega}) \), for a \( \langle f | H_\gamma | i \rangle \) matrix element for a final (initial) many-body state, \( f \) (\( i \)). A previous study used self-consistent methods to show that \( \chi \) decreases with \( N_\omega \), to leading order in \( \lambda_\omega / N_\omega \) [162]. This approximation has also been used in a previous Sp(3, \( \mathbb{R} \))-based study of cluster-like states of \( ^{16}\text{O} \) [163]. The average contribution \( \langle Q \cdot Q \rangle_{N_n} \) of \( Q \cdot Q \) for a given number of \( N_n \) HO excitations [164] introduces a considerable renormalization of the HO shell structure and hence is removed in multishell studies [165].

The only adjustable parameter in the interaction is \( \gamma \), which introduces into the model hierarchical many-body interactions in a prescribed way. One can see this through a polynomial expansion of the exponential in Eq. (3.13), which also parallels the interaction used in Ref. [166], that was applied to the \( ^{24}\text{Mg} \) ground state rotational band. In particular, in considering this expansion, we find that higher-order terms in \( Q \cdot Q \) of Eq. (3.13) become quickly negligible for a reasonably small \( \gamma \). For example, for the ground state of \( ^{12}\text{C} \), it is sufficient to include only the \( Q \cdot Q \) and \( (Q \cdot Q)^2 \) terms. For more deformed systems, such as the Hoyle state in \( ^{12}\text{C} \), however it is necessary to include terms up through \( (Q \cdot Q)^4 \) (third order in \( \gamma \)) in the expansion [109].

### 3.2.2 Model Spaces

In this study, we consider various model spaces for \( ^{12}\text{C} \) consisting of symplectic irreps with bandheads of large quadrupole deformation and low intrinsic spin (Table 3.1), which allows results to be examined for convergence. Following the symmetry-guided concept, we first consider a model space consisting of the most deformed spin-0 \( 0h\Omega \), \( 2h\Omega \), and \( 4h\Omega \) bandheads together with their symplectic excitations up through \( N_{\max} = 20 \) with total dimensionality of \( 4.5 \times 10^3 \) (\( \mathcal{C}-1 \) in Table 3.1). Then, the model space is expanded “horizontally” through the inclusion of higher-lying bandheads and bandheads of decreasing deformation to model spaces \( \mathcal{C}-2 \) (with total dimensionality of \( 6.6 \times 10^3 \), \( \mathcal{C}-3 \) and \( \mathcal{C}-4 \). The \( \mathcal{C}-4 \) selection, for
example, includes the symplectic irreps 0\(h\Omega(04), 4h\Omega(120), 2h\Omega(62)\) and 6\(h\Omega(102)\) that have been identified to have the lowest mean-field energy based on shape-consistent mean-field considerations [158]. We also consider the model space that includes all Sp(3, \(\mathbb{R}\)) irreps with low spin, spin-0 and spin-1, 0\(h\Omega\) bandheads with symplectic excitations up to \(N_{\text{max}} = 20\) (\(\mathcal{C}-5\) in Table 3.1). This space consists of the complete 0\(h\Omega\) model space for \(^{12}\text{C}\), excluding only the spin-2 part of the (20) 0\(h\Omega\) configuration, which is expected to be influenced by a spin-2 interaction, such as a tensor force [167, 168]. Given the spin-0 and spin-1 nature of the model interaction we use, inclusion of the tensor force is outside of the scope of the present model, but will be considered in future studies. Nonetheless, as discussed next, the model interaction has been shown to yield results for \(A = 8\) to \(A = 24\) in close agreement with \textit{ab initio} studies and experiment [109, 118, 119], with model space selections as small as \(\mathcal{C}-1\) and \(\mathcal{C}-2\) found to be sufficient.

Table 3.1: Sp(3, \(\mathbb{R}\)) irreps (specified by their bandhead labels) included in each of the model spaces considered. Each of model spaces \(\mathcal{C}-1\) through \(\mathcal{C}-4\) includes its preceding model space, while model space \(\mathcal{C}-5\) expands \(\mathcal{C}-2\) by including all spin-0 and spin-1 0\(h\Omega\) bandheads, which are, in fact, all the SU(3) configurations that exist in the 0\(h\Omega\) subspace. All model spaces extend up to \(N_{\text{max}} = 20\).

<table>
<thead>
<tr>
<th>Model Space</th>
<th>0(h\Omega)</th>
<th>2(h\Omega)</th>
<th>4(h\Omega)</th>
<th>6(h\Omega)</th>
<th>8(h\Omega)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\mathcal{C}-1)</td>
<td>(0 4)</td>
<td>(6 2)</td>
<td>(120)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\mathcal{C}-2)</td>
<td>(0 4)</td>
<td>(12)</td>
<td>(62)</td>
<td>(120)</td>
<td></td>
</tr>
<tr>
<td>(\mathcal{C}-3)</td>
<td>(0 4)</td>
<td>(12)</td>
<td>(62)</td>
<td>(120)</td>
<td>(140)</td>
</tr>
<tr>
<td>(\mathcal{C}-4)</td>
<td>(0 4)</td>
<td>(12)</td>
<td>(62)</td>
<td>(120)</td>
<td>(140)</td>
</tr>
<tr>
<td>(\mathcal{C}-5)</td>
<td>(0 4)</td>
<td>(20)</td>
<td>(0 1)</td>
<td>(62)</td>
<td>(120)</td>
</tr>
</tbody>
</table>

3.2.3 Comparison to \textit{Ab Initio} Results

Before discussing results of this model, we compare the ground state wave function calculated in the NCSpM to current results for \(^{12}\text{C}\) within an \textit{ab initio} framework. In order to
make this comparison, results are shown for smaller model spaces, for which \textit{ab initio} NCSM calculations are feasible. For the ground state (gs) rotational band, the $N_{\text{max}}=6$ model space appears to be reasonable for both models (Fig. 3.2). In particular, we compare to wave functions obtained in the SA-NCSM [122] with the bare JISP16 realistic interaction [169]. In these calculations, the SA-NCSM utilizes an SU(3)-coupled basis, which yields eigenfunctions equivalent to the conventional NCSM wave functions [121], but realized in terms of the $(\lambda \mu)$ deformation labels, and hence, the deformed configurations that dominate the $^{12}\text{C}$ wave functions can be straightforwardly studied. The SA-NCSM is not limited to the SU(3) basis: it has been implemented in other studies within an $\text{Sp}(3,\mathbb{R})$ basis as well [123].

Figure 3.2: Probability distribution for $^{12}\text{C}$ across the $N_n$ total excitations of the lowest $0^+$ state as calculated by the NCSpM with $H_\gamma$ (left bars) using the $\text{C}-2$ model space. This distribution is compared to the \textit{ab initio} SA-NCSM with the bare JISP16 NN interaction (right bars). Both models are limited to an $N_{\text{max}}=6$ model space for comparison. The dominant shapes, specified by $(\lambda \mu)$, are shown, and contributions are organized according to their proton, neutron, and total spin $S_pS_nS$. See Fig. 1 in Ref. [110] for a comparison of the $4^+_1$ wave functions, and further discussion.

Consistent with the outcome of Refs. [122] and [119] (see, e.g., Fig. 1 in Ref. [122] for $^6\text{Li}$ and $^8\text{Be}$ wave functions in $N_{\text{max}}=8$-10), the \textit{ab initio} $N_{\text{max}}=6$ SA-NCSM results with the bare JISP16 realistic interaction for the $0^+$ gs, first $2^+$, and first $4^+$ states of $^{12}\text{C}$ reveal the dominance of the $0\hbar\Omega$ component with the foremost contribution coming from the leading $|\sigma = 0(04), S = 0\rangle$ irrep, where $S=0$ is the total spin of the state (see Fig. 3.2 for the gs wave
function). Important SU(3) configurations are then organized into structures that follow the Sp(3, R) symplectic symmetry. Notice, for example, that this (0 4) symplectic irrep gives rise to dominant (0 2) and (2 4) configurations in the 2ℏΩ subspace and so on (see Fig. 3.2, solid blue bars), and those configurations realize the major components of each of the wave functions in this subspace. The next most important configuration is the \(|0(1 2)S = 1\rangle\) irrep, with its associated symplectic excitations (Fig. 3.2, striped purple bars). Among all possible configurations present in the SA-NCSM (total of \(1.26 \times 10^6\) for \(J = 0\) in \(N_{\text{max}}=6\)), only the states belonging to the (0 4) and the (1 2) symplectic irreps appear dominant. This further confirms the significance of the symplectic symmetry to nuclear dynamics: the outcome points to the fact that the relevant model space can be systematically determined by down-selecting to important spin configurations in lower subspaces while expanding to include a manageable set of symplectic configurations in the higher \(N_{\text{max}}\) regime.

Furthermore, we find a close similarity between complete \textit{ab initio} SA-NCSM results and the NCSpM wave functions of the \(^{12}\text{C}\) gs rotational band, calculated with \(H_\gamma\) of Eq. (3.13) for \(\gamma = 1.71 \times 10^{-4}\) and symplectic irreps of model space \(\mathfrak{C}-2\) (Fig. 3.2). NCSpM and SA-NCSM calculations are performed for \(h\Omega = 18\) and an \(N_{\text{max}}=6\) model space. The two models show close agreement of the probability distribution, including the SU(3) content of the wave functions. This suggests that the interaction used in the NCSpM has effectively captured a major portion of the underlying physics of the realistic interaction important to the low-lying nuclear states.

### 3.2.4 NCSpM Results: \(^{12}\text{C}\)

Using this interaction, then, we determine the low-lying energy spectrum of \(^{12}\text{C}\), as well as other important observables, including electromagnetic transitions, matter \(rms\) radii, and quadrupole moments.

The NSCpM utilizes Bahri’s symplectic computational code [170], which uses Draayer & Akiyama’s SU(3) package [171]. The symmetry-mixing spin-orbit term is calculated in
Figure 3.3: Energy spectrum for $^{12}$C calculated using the NCSpM with symplectic irreps starting at 0p-0h (blue, left), 2p-2h (green, center), and 4p-4h (red, right) bandheads and extending to $N_{\text{max}} = 20$, for model spaces $\mathcal{C}-1$ and $\mathcal{C}-2$. Experimental data is from [172], except the latest results for $0^+_{\text{3}}$ [173] and the states above the Hoyle state, $2^+_{\text{2}}$ [174] and $4^+_\text{4}$ [175]. The $B(E2; J \rightarrow J-2)$ transition rates are in W.u. with theoretical uncertainties estimated for a $\pm 60\%$ deviation of the Hoyle-state energy. Spectra calculated in model spaces $\mathcal{C}-3$ and $\mathcal{C}-4$ are the same as those shown for model space $\mathcal{C}-2$.

The model successfully reproduces the ground-state and Hoyle-state rotational bands in $^{12}$C [109]. Both rotational features and $\alpha$-cluster substructures are shown to emerge in the fully microscopic $N_{\text{max}} = 20$ no-core shell-model framework, as suggested by the reasonably close agreement of the model outcome with experiment and ab initio results in smaller spaces. While the model includes an adjustable parameter, $\gamma$, this parameter only controls the presence of many-nucleon interactions, and hence, introduces an additional, but very limited, degree of freedom. The entire many-body apparatus is fully microscopic and no adjustments are possible. We find that, as $\gamma$ varies, there is only a small window of possible
\( \gamma \) values around \( \gamma = 1.71 \times 10^{-4} \) which, for large enough \( N_{\text{max}} \), closely reproduce the relative positions of the three lowest \( 0^+ \) states in \(^{12}\text{C}\) and associated measured observables, discussed below. The model has been also applied to low-lying states of other nuclei, such as \(^{8}\text{Be}\) and \(sd\)-shell nuclei [118,119], without any further parameter adjustment. In particular, using the same \( \gamma = 1.71 \times 10^{-4} \), we have described selected low-lying states in \(^{8}\text{Be}\) in an \( N_{\text{max}} = 24 \) model space with only 3 spin-0 \( 0\hbar\Omega \) (0 4), \( 2\hbar\Omega \) (6 0), and \( 4\hbar\Omega \) (8 0) symplectic irreps [119], as well as the ground-state rotational band of heavier nuclei, such as \(^{20}\text{O}\), \(^{20,22,24}\text{Ne}\), \(^{20,22}\text{Mg}\), and \(^{24}\text{Si}\), using \( N_{\text{max}} = 12 \) model spaces [118].

### 3.2.5 Clustering and Collectivity from a Many-Body Perspective

In this section, we focus on the ground state and Hoyle state in \(^{12}\text{C}\), along with their rotational bands. We begin with a study of the dependence of the NCSpM results on the model space and the model parameters \( \gamma \). As described above, we use \( H_\gamma \) with \( \gamma = 1.7\times10^{-4} \), \( \hbar\Omega = 18 \text{ MeV} \), and \( \kappa = 3.8 \text{ MeV} \). We also discuss how the current study gives strong evidence that the NCSpM, with its use of the symplectic symmetry, is uniquely positioned to reveal clustering phenomena in cluster-like systems, such as the Hoyle state of \(^{12}\text{C}\).

Analysis of the results shows that model space \( \mathcal{C}-1 \), consisting of irreps built upon the spin-0 \( 0\hbar\Omega \) 0p-0h (0 4), the \( 2\hbar\Omega \) 2p-2h (6 2), and the \( 4\hbar\Omega \) 4p-4h (12 0) bandheads, is capable of bringing the Hoyle state down in energy (Fig. 3.3, last column). For this model space, we observe three low-lying \( 0^+ \) states below 10 MeV, and their rotational bands (e.g., \( 0^+, 2^+, \) and \( 4^+ \)): the 0p-0h ground state (Fig. 3.3, first column), the 4p-4h \( 0^+ \) state that tracks with the Hoyle state, and a 2p-2h (Fig. 3.3, middle column) above the 4p-4h \( 0^+ \) state. However, this model space yields a compressed energy spectrum. We note that the spin-orbit interaction, being a tensor operator of spin 1, does not mix spin-0 irreps. Hence, for this model space, the spin-orbit term has no effect (equivalent to \( H_\gamma \) with \( \kappa = 0 \)) and the \( H_\gamma \) eigenstates consist of a single symplectic irrep.

With the expansion of the model space by only one spin-1 irrep (model space \( \mathcal{C}-2 \)), the
$N_{\text{max}} = 20$ NCSpM energy spectrum is improved and found to lie reasonably close to the experimental data (Fig. 3.3, see C-2) [109]. The $\text{Sp}(3,\mathbb{R})$-nonpreserving spin-orbit term mixes the spin-0 (0 4) and spin-1 (1 2) irreps for all $J^x = 0^+$, $2^+_1$, and $4^+_1$, which results in a more realistic energy spacing between the excited states. Specifically, we see the $gs$ separating from the higher-lying $0^+$ states, and a slight stretching in the $gs$ rotational band. This agrees with early cluster models that showed similarly compressed spectra, which were corrected through allowing for $\alpha$-cluster dissociation due to a spin-orbit force, as discussed in Ref. [114]. The inclusion of this additional irrep introduces another low-lying 0p-0h $0^+$ state (Fig. 3.3, first column), which – along with the 2p-2h $0^+$ state – lies close to the broad $0^+$ resonance at 10 MeV, observed in $^{12}\text{C}$.

In the present model, the spin-orbit interaction is turned on only among the bandheads of the symplectic irreps, up to $N_{\text{max}} = 4$ for the C-2 model space (and $N_{\text{max}} = 8$ for C-4), which results in the mixing of basis states within $S = 0$ and $S = 1$ irreps up to $N_{\text{max}} = 20$ (see the NCSpM results shown in Fig. 3.2 for $N_{\text{max}} = 6$ and the $^{12}\text{C}$ ground state). These calculations are performed in the SA-NCSM, referenced above, which is ideal for the symplectic bandheads under consideration, because they are equal to the corresponding SU(3) basis states of the SA-NCSM. The full accounting of the spin-orbit interaction is estimated, at the most, to render additional mixing of about 0.2% for (6 2), $4 \times 10^{-4}\%$ for (12 0), and 11% for (1 2) and (0 4) to the $^{12}\text{C}$ $gs$, while increasing the corresponding $0^+$ state energies by only a few MeV without affecting their order. That the bandheads provide a reasonable account of the spin-orbit effect stems from an important feature of the $l \cdot s$ operator – it is a spin-1 $0h\Omega(1 1)$ SU(3) tensor and only mixes certain configurations within the irreps. Specifically, the main contribution to the spin-orbit matrix elements between the (1 2) irrep and the (6 2) irrep, or the (12 0) irrep, comes from higher-$N_n$ configurations where the (1 2) probability amplitudes are already small, 1-8% (see Fig. 3.2). In addition, mixing to the (6 2) and (12 0) irreps is not allowed by SU(3) selection rules for the most dominant configurations in these irreps, and it involves only configurations of probability amplitudes...
Table 3.2: Transition rates, $B(E2)$ in W.u. and $M(E0)$ in $e$ fm$^2$, as well as rms matter radii ($r_{rms}$) in fm and the electric quadrupole moment in $e$ fm$^2$ obtained by the NCSpM with $H_γ$ in model spaces $\mathcal{C}$-1 and $\mathcal{C}$-2 (with $\mathcal{C}$-2 results coinciding with those for model spaces $\mathcal{C}$-3 & $\mathcal{C}$-4), as well as for a 1.7% mixing of the $(12\,0)$ irrep into the $(0\,4)$ irrep (see text for details). Experimental values are shown in the rightmost column.

<table>
<thead>
<tr>
<th></th>
<th>$\mathcal{C}$-1</th>
<th></th>
<th>$\mathcal{C}$-2</th>
<th></th>
<th>Expt.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NCSpM Mixing</td>
<td>NCSpM</td>
<td>NCSpM Mixing</td>
<td>NCSpM</td>
<td>Ref. [172]</td>
</tr>
<tr>
<td>$B(E2; 2_1^+ \rightarrow 0_{gs}^+$)</td>
<td>5.12 4.37</td>
<td>4.3 3.64</td>
<td>4.65(26)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$B(E2; 0_2^+ \rightarrow 2_1^+$)</td>
<td>0 8.7 0 8.4</td>
<td>8.0(11)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$B(E2; 2_2^+ \rightarrow 0_{ gs}^+$)</td>
<td>63.2 60.5</td>
<td>63.2 60.5</td>
<td>N/A</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$M(E0; 0_2^+ \rightarrow 0_{gs}^+$)</td>
<td>0 2.04</td>
<td>0 2.1</td>
<td>5.4(2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$r_{rms}$ $0_{ gs}^+$</td>
<td>2.44 2.45</td>
<td>2.43(1) 2.44</td>
<td>2.43(2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$r_{rms}$ $0_2^+$ (Hoyle)</td>
<td>2.93 2.92</td>
<td>2.93(5) 2.92</td>
<td>2.89(4)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$Q_{2_1^+}$</td>
<td>6.63 6.17</td>
<td>5.9(1) 5.44</td>
<td>+6(3)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

of less than 0.5% for $(6\,2)$ and 0.02% for $(12\,0)$. This results in negligible effects on the states and associated energies. In addition, the bandheads of the $(0\,4)$ and $(1\,2)$ irreps constitute a major component of the wave functions, which is $\sim 70\%$ of the $0_{ gs}^+, 2_1^+, \text{and } 4_1^+$ states.

Of particular note is the $2^+$ state, calculated by the NCSpM as a rotational excitation 1.51 MeV above the second $0^+$ state (see Fig. 3.3, last column). Morinaga was the first to suggest that this $2^+$ state, which he estimated to be at 9.7 MeV, could be a member of a Hoyle-state rotational band [40]. The existence of a $2^+$ state near this energy has important implications for astrophysical reaction rates [176], and has been the subject of many experimental studies since Morinaga first suggested it as a mechanism to probe the structure of the Hoyle state. More recent experimental studies have given rise to much debate surrounding the $2^+_2$ state: inelastic $^{12}$C$(\alpha, \alpha')$ and $^{12}$C$(p, p')$ scattering reactions showed evidence for an excited $2^+_2$ around 9.6-11 MeV [173, 174, 177, 178], but studies of the $\beta$-decay of $^{12}$N and $^{12}$B found no evidence for the existence of a $2^+$ state below 10 MeV [179, 180]. The NCSpM first identified a low-lying $2^+$ state as a part of the $0_{gs}^+$ rotational band at 10.68 MeV [119], which used model space $\mathcal{C}$-1 and a rescaling factor. A subsequent study used the $^{12}$C$(\gamma, \alpha_0)^8$Be reaction ($\alpha_0$ indicates that the reaction takes place through the $0^+$ state in $^8$Be), and identified
the $2^+_2$ state at 10.03(11) MeV with a total width of 800(130) keV [174], or approximately 2.4 MeV above the Hoyle-state energy. For comparison, recent \textit{ab initio} $N_{\text{max}} = 8$ NCSM calculations, while achieving a remarkable reproduction of the $gs$ rotational band, yield the second low-lying $0^+$ and $2^+$ states around 13 MeV and 15 MeV, respectively [181], which are thus believed to be associated with higher-lying states of spin-parity $0^+$ and $2^+$. Here, we also identify a low-lying $4^+$ state at 11.7 MeV (see Fig. 3.3), which tracks with experimental identification of a low-lying $4^+$ state believed to be in the Hoyle-state rotational band [175].

The NCSpM is also used to study observables of $^{12}\text{C}$, such as $B(E2)$ transition strengths, $Q_{21^+}$ electric quadrupole moments, and matter rms radii for the $gs$ and Hoyle state. A comparison of results for model spaces \( \mathcal{C}-1 \) and \( \mathcal{C}-2 \) (see columns 2 and 4 in Table 3.2) shows slight differences, implying that the spin-orbit interaction has only a small effect on these observables. While the in-band transition strengths are quite reasonable, a nonzero $B(E2; 0^+_2 \rightarrow 2^+_1)$ value can only result from mixing of symplectic irreps, which requires an interaction with an $\text{Sp}(3, \mathbb{R})$ symmetry-breaking term beyond the spin-orbit interaction. To examine a possible mixing of the $4p-4h$ ($120$) irrep into the ground state, we consider an ad-hoc mixing of the $0p-0h$ and $4p-4h$ irreps, which is equally applied to all the states within each irrep. However, we find that an extremely small mixing, 1.7%, of the ($120$) irrep into the $0p-0h$ irreps of the $gs$ rotational band is sufficient to realize the observed $B(E2)$ rates and to yield results consistent with the $M(E0)$ experimental value (Table 3.2). The results indicate that while the mixing has some effect on the collectivity within the $gs$ rotational band, the matter rms radii for the ground and Hoyle states remain unaffected.

**Dependence on horizontal expansion** – As shown above, reasonable results for $^{12}\text{C}$ are obtained using the \( \mathcal{C}-2 \) model space. We examine a possible dependence of the outcome as more symplectic irreps are added into the model space by considering \( \mathcal{C}-3 \) and \( \mathcal{C}-4 \) (Table 3.1). This leads to more configurations within each “horizontal” HO shell. We find that all the \( \mathcal{C}-2 \) results presented in Fig. 3.3 and Table 3.2 remain unaltered, and that no additional low-lying $0^+$ states are introduced to the $^{12}\text{C}$ spectrum with the inclusion of the most deformed
Table 3.3: Low-lying $0^+$ states calculated as the lowest $0^+$ state for each $\text{Sp}(3, \mathbb{R})$ irrep specified by its bandhead in the table and for the model spaces $\mathcal{C}-3$ and $\mathcal{C}-4$ (see Table 3.1). Energies are reported with respect to the ground state in MeV. For comparison, the Hoyle-state energy given by the lowest $0^+$ state within the $4\hbar\Omega(120)$ irrep is 6.66 MeV.

<table>
<thead>
<tr>
<th>$N_{\sigma}(\lambda_{\sigma} \mu_{\sigma})$</th>
<th>$\mathcal{C}-3$</th>
<th>$\mathcal{C}-4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2\hbar\Omega(24)$</td>
<td>30.68</td>
<td></td>
</tr>
<tr>
<td>$4\hbar\Omega(8.2)$</td>
<td>31.94</td>
<td></td>
</tr>
<tr>
<td>$4\hbar\Omega(4.4)$</td>
<td>55.61</td>
<td></td>
</tr>
<tr>
<td>$4\hbar\Omega(0.6)$</td>
<td>70.53</td>
<td></td>
</tr>
<tr>
<td>$6\hbar\Omega(140)$</td>
<td>34.21</td>
<td>34.21</td>
</tr>
<tr>
<td>$6\hbar\Omega(102)$</td>
<td>57.56</td>
<td></td>
</tr>
<tr>
<td>$8\hbar\Omega(160)$</td>
<td>63.12</td>
<td>63.12</td>
</tr>
</tbody>
</table>

$S = 0$ bandheads at $6\hbar\Omega$ and $8\hbar\Omega$ as in model space $\mathcal{C}-3$, nor with the inclusions of $S = 0$ bandheads of decreasing deformation, as in model space $\mathcal{C}-4$ (Table 3.3). Thus, we find the results to be converged with respect to a horizontal expansion of the model space. Model space $\mathcal{C}-5$ does produce an additional low-lying, $(20)$-dominated $0^+$ state below the Hoyle-state energy. A similar state appears at 15 MeV in $\textit{ab initio}$ SA-NCSM calculations for the complete $N_{\text{max}} = 8$ model space. However, with a radius almost equal to that of the ground state (2.41 fm) and a very weak monopole transition strength ($0.29 \text{ efm}^2$), this is not a viable candidate for the Hoyle state.

**Dependence on vertical expansion** – A study of the effect of the $N_{\text{max}}$ cutoff on the convergence of $B(E2)$ [Fig. 3.4(a) and 3.4(b)] shows that, for both model spaces $\mathcal{C}-1$ and $\mathcal{C}-2$, large $N_{\text{max}}$ values are required in order to reach convergence. Indeed, we find that, while convergence for the $gs$ rotational band is achieved around $N_{\text{max}} = 12$, the Hoyle-state rotational band requires at least $N_{\text{max}} = 18$ for convergence. Similar dependence on $N_{\text{max}}$ is found for the matter rms radius of the ground state and for the electric quadrupole moment [Fig. 3.4(c) and 3.4(d), respectively], both of which require at least $N_{\text{max}} = 12$ for convergence. The dependence on $N_{\text{max}}$ does not improve with inclusion of additional symplectic irreps; that is, convergence cannot be achieved with low $N_{\text{max}}$ and many symplectic irreps. These observations underscore the importance of high $N_{\text{max}}$ values for achieving converged...
Figure 3.4: Dependence of NCSpM (γ = 1.71 × 10^{-4}) on $N_{\text{max}}$ for (a) $B(E2)$ of the $gs$ rotational band in model spaces $\mathcal{C}$-1 and $\mathcal{C}$-2 (see Table 3.1), as well as (b) $B(E2)$ of the Hoyle-state rotational band, (c) $gs$ point-particle matter rms radius, and (d) the electric quadrupole moment for $2^+_1$ in model space $\mathcal{C}$-2 (with results for $\mathcal{C}$-3 and $\mathcal{C}$-4 identical to those of $\mathcal{C}$-2).
Figure 3.5: Dependence of the $^{12}$C NCSpM energy spectrum on the $\gamma$ model parameter for $N_{\text{max}} = 20$ in model space C-2 (see Table 3.1). Available experimental values are shown for (b), (c), and (d) and compared to the NCSpM results quoted in Table 3.2 for $\gamma = 1.71 \times 10^{-4}$.

**B(E2)** strengths. Such $N_{\text{max}}$ values are within reach of the NCSpM but well-beyond that of the NCSM calculations due to the combinatorial growth of its model spaces with increasing $N_{\text{max}}$ values.

**Dependence on model parameters** – The strength parameter $\gamma$ effectively determines to what extent higher-order many-body interactions will contribute to the calculation. A study of its effect on the $^{12}$C energy spectrum [Fig. 3.5(a)] reveals that the additional degree of freedom associated with the $\gamma$ model parameter is substantially limited by the lowest $0^+$ states (with only a small effect on the gs rotational band). Indeed, given the dramatic variation with $\gamma$ for the $0^+_2$ and $0^+_3$ levels, there is only a small range of reasonable $\gamma$ values. In this range, energies and other observables, such as rms matter radii, $B(E2)$ transition rates, and the electric quadrupole moment [see Fig. 3.5(b)-(d), respectively], are found to be in agreement with experiment. As the $\gamma$ value decreases from the value adopted in this model (with a limit $\gamma \to 0$, for which the NCSpM simplifies to a multi-shell Elliott model), higher-shell excitations become energetically more favorable and the nucleus expands spatially. This
Figure 3.6: NCSpM probabilities and amplitudes (insets) for (a) the ground-state rotational band, (b) the Hoyle-state rotational band, and (c) the GMR and GQR for $^{12}$C. States with probabilities $\geq 0.1\%$, which make up 98.83\% − 99.63\% of the wave functions, are included in the figures.
is accompanied by enhancement of collectivity and by considerably larger $B(E2)$ transition strengths. Hence, the second and third $0^+$ states of large deformation fall below the $0^+_{gs}$ state for small values of $\gamma$ [Fig. 3.5(a)]. In the limit $\gamma \to \infty$, the Hamiltonian becomes a HO potential plus a spin-orbit force. In this case, lowest-energy configurations are favored, and the energy of the 2p-2h state is about $2\hbar\Omega$ MeV lower than that of the 4p-4h state. It is then remarkable that for the value of the $\gamma$ parameter adopted in this study – which yields reasonable reproduction of the Hoyle state – energy spectra and other observables in $p$- and $sd$-shell nuclei are found in a reasonable agreement with their experimental counterparts without further adjustment [118,119].

The spin-orbit strength $\kappa$ is selected using an empirical estimate (see Sec. 3.2.1), and is not adjusted in the present calculations. However, a $\pm 20\%$ variation of the $\kappa$ parameter shows changes of less than $\pm 1$ MeV for states in the low-lying energy spectrum (see inset of Fig. 4a in Ref. [109]), and has no considerable effect on the other observables under consideration (0.05% to 3%).

### 3.2.6 Deformation and Giant Resonances

Important information about deformation is found through analysis of the SU(3) $(\lambda\mu)$ configurations that comprise the NCSpM wave function. This is based on an established mapping [155,159,182] between the SU(3) $(\lambda\mu)$ labels and the shape variables used in the Bohr-Mottelson collective model [161]. In particular, for large deformation, the labels $(\lambda 0)$ and $(0 \mu)$ can be associated with distinctly prolate and oblate shapes, respectively. From this, it is clear that, while the predominant component of the lowest $0^+$ state in $^{12}$C is at $0\hbar\Omega$ and manifests an evident oblate shape [Fig. 3.6(a)], the second $0^+$ state (Hoyle state) peaks around $8\hbar\Omega$ with a clear indication of a prolate shape deformation, with $(16 0)$ being the largest contribution [Fig. 3.6(b)]. The strong prolate deformation of this $0^+_2$ state together with the significance of the 4p-4h symplectic irrep (built on a configuration of three alpha particles, each occupying a single HO shell) indicate that this $0^+$ state has an
Table 3.4: Energies in MeV of the first excited $0^+$ state, $E_{\text{GMR}}$, and the lowest excited $2^+$ state that peaks above $0\hbar\Omega$, $E_{\text{GQR}}$, within the ground-state symplectic irrep for selected $p$- and $sd$-shell nuclei, and their associated $B(E2)$ transition rates in W.u., $B(E2;\uparrow)$ for $0_{\text{GMR}}^+ \rightarrow 2^+_1$ and $B(E2;\downarrow)$ for $2_{\text{GQR}}^+ \rightarrow 0^+_{gs}$, calculated with the NCSpM using model space $\mathcal{C}$-1.

<table>
<thead>
<tr>
<th></th>
<th>$E_{\text{GMR}}$ (MeV)</th>
<th>$B(E2;\uparrow)$ (W.u.)</th>
<th>$E_{\text{GQR}}$ (MeV)</th>
<th>$B(E2;\downarrow)$ (W.u.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{12}\text{C}$</td>
<td>27.90</td>
<td>2.38</td>
<td>20.87</td>
<td>7.43</td>
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<tr>
<td>$^{16}\text{O}$</td>
<td>29.35</td>
<td>21.94</td>
<td>23.54</td>
<td>8.13</td>
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<tr>
<td>$^{20}\text{O}$</td>
<td>23.61</td>
<td>6.82</td>
<td>23.40</td>
<td>3.58</td>
</tr>
<tr>
<td>$^{20}\text{Mg}$</td>
<td>23.61</td>
<td>15.35</td>
<td>23.40</td>
<td>8.05</td>
</tr>
<tr>
<td>$^{20}\text{Ne}$</td>
<td>24.27</td>
<td>11.94</td>
<td>24.39</td>
<td>5.90</td>
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<td>$^{22}\text{Mg}$</td>
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<td>$^{22}\text{Ne}$</td>
<td>25.17</td>
<td>9.14</td>
<td>24.97</td>
<td>4.46</td>
</tr>
</tbody>
</table>

underlying alpha-particle cluster structure. This points to a need for next-generation NCSM models, which are capable of $ab\ initio$ calculations in larger model spaces, in order to capture important structural information for the Hoyle state.

In light nuclei, both the giant monopole resonance (GMR) and giant quadrupole resonance (GQR) are expected to be broad resonances, of width a few hundred keV, and are particularly difficult to identify experimentally because of their large overlap with other multipolarities (see, e.g., [183]). The GMR is understood to be the first $0^+$ excitation of the $gs$ symplectic irrep [184], which is a breathing mode with a similar shape to that of the ground state [see Fig. 3.6(c) for $^{12}\text{C}$]. The GQR candidates are identified as part of the $gs$ symplectic irrep as the lowest excited $2^+$ state that peaks above $0\hbar\Omega$ (Table 3.4). For example, for $^{20}\text{Mg}$, the $gs$ symplectic irrep adopted is the one that builds upon the most deformed $0\hbar\Omega$ configuration $(4\,2)$ – for this irrep, the first excited $0^+$ state has a broad peak with its maximum at $2\hbar\Omega$ with $(6\,2)$ being the most dominant contribution, while the third $2^+$ state exhibits a broad peak with a dominant $2\hbar\Omega(6\,2)$ configuration (note that the two lowest $2^+$ states for this irrep peak at $0\hbar\Omega$ and are part of the $gs$ rotational band). These
dominant configurations represent excitations of the symplectic bandhead induced by the $A^{(20)}_L$ symplectic generators with $L = 0$ for the GMRs (or equally, by the monopole operator) and $L = 2$ for GQRs (or equally, by the quadrupole operator). In general, the main contributions to both GMRs and GQRs arise from excitations described by multiples of the $A^{(20)}_L$ operators. For $^{12}$C, both the GMR and GQR have non-negligible contributions up to $N_{\text{max}} = 14$ [Fig. 3.6(c)]. Because the giant resonances are very broad in light nuclei, the inclusion of higher $N_{\text{max}}$ configurations is critical for describing their structure.

Previous studies of the GQR for $^{16}$O in the symplectic framework identify the resonance near $E_x = 25$ MeV with a $B(E2; \downarrow) \approx 17 e^2 f m^4$ or 10 W.u. [185]. The NCSpM corroborates these results (Table 3.4): it identifies the second $2^+$ excitation of the $gs$ symplectic irrep of $^{16}$O at 23.54 MeV as having a similar dominant $2\hbar \Omega$ 1p-1h configuration, with a strong $B(E2)$ transition to the ground state. Analysis of the GMR and GQR candidates for a selection of $p$- and $sd$-shell nuclei shows the two resonances close in energy, with a typically higher energy for the breathing mode. Notably, the oblate GMR for $^{12}$C appears much higher in energy than the prolate 4p-4h deformed state near the Hoyle-state energy.

Given its success in reproducing highly clustered states, as in the Hoyle state, as well as clustering and collective features such as electromagnetic transitions, matter $rms$ radii, and giant resonances, it stands to reason that the symplectic symmetry is a strong candidate for use in nuclear reaction theory. In the following Chapter, we will discuss nuclear reactions from a few-body perspective, before deriving (in Chapter 5) a many-body nuclear reaction theory that capitalizes on the benefits of the symplectic symmetry for reproducing clustering and collectivity.
4 Nuclear Reactions: Background and Theoretical Tools

With this chapter, we introduce fundamental terminology and concepts in the study of nuclear reactions, discuss the different ways in which nuclear reactions are categorized, and motivate the study of reactions in each of these categories. We connect nuclear observables with a few-body picture of nuclear dynamics, and discuss observables we intend to calculate in the following chapters, including reaction rates, partial widths, and ANCs.

4.1 Common Terms and Definitions for Reaction Theory

Low-energy nuclear reactions typically involve a target nucleus $A$, a projectile $a$, some number of observed ejectiles, and a remnant or residual nucleus $C$. We can indicate nuclear reactions in a number of ways. For example, the capture of an alpha particle on $^{16}\text{O}$ can be written as $^{16}\text{O} + \alpha \rightarrow ^{20}\text{Ne}^*$ or $^{16}\text{O}(\alpha, \gamma)^{20}\text{Ne}$.

When talking about nuclear reactions, we often identify entrance and exit channels and partitions. Within the scope of this paper, the entrance partition, for example, refers to how the particles involved in the reaction are separated into clusters before the reaction takes place. For example, when we talk about alpha capture on $^{16}\text{O}$, the entrance partition is $^{16}\text{O} + \alpha$, and two possible exit partitions are $^{20}\text{Ne}$ and $^{19}\text{Ne} + n$. A channel defines specific quantum numbers of a partition: for the $^{16}\text{O} + \alpha$ reaction, $1^-$ is a particular exit channel of the $^{20}\text{Ne}$ exit partition. In other studies, one can find the term “channel” used both to describe a channel or partitioning (for the sake of clarity, we distinguish between the two).

4.1.1 Classifying Nuclear Reactions

One important defining characteristic of nuclear reactions is the $Q$-value, which is the amount of energy stored or released in a reaction, determined by the mass difference in the entrance and exit partitions. The total energy in the entrance and exit channels must be conserved. For the reaction $A + a \rightarrow C + c$, where the target $A$ is assumed to be stationary, the projectile $a$ has kinetic energy $T_a$, the residual $C$ has kinetic energy $T_C$, and the ejectile
\( c \) has kinetic energy \( T_c \), the conservation of energy is given by

\[
M_A + M_a + T_a = M_C + M_c + T_C + T_c
\]

\[
M_A + M_a - (M_C + M_c) = T_C + T_c - T_a,
\]  
\( (4.1) \)

for masses in MeV. The \( Q \)-value, given by,

\[
Q = M_A + M_a - (M_C + M_c),
\]  
\( (4.2) \)

thus encodes the difference in the kinetic energy in the entrance and exit partitions. \textit{Exothermic} reactions have \( Q > 0 \) MeV, meaning they release energy, and \textit{endothermic} reactions have \( Q < 0 \) MeV, and so they require energy input to take place.

There are a number of ways in which one can classify low-energy reactions, in addition to whether energy is produced or consumed in the process. One can also classify low-energy reactions based on (1) the observed entrance and exit channels, and (2) the number of excited degrees of freedom. The former method compartmentalizes reactions into a large number of categories: elastic scattering reactions, inelastic scattering reactions, knock-out reactions, capture reactions, breakup reactions, charge exchange reactions, and transfer reactions which are further separated into stripping and pickup reactions. Table 4.1 describes the differences in these categorizations.

The second classification scheme, based on the number of excited degrees of freedom, categorizes reactions as either \textit{direct} or \textit{compound}. Direct reactions happen relatively quickly and at higher energies, with little momentum transfer. They involve only single-particle excitations within the target, and few collisions between the projectile and nucleons in the target. They tend to leave the target nucleus intact. In direct reactions, the exit channel has a “memory” of the entrance channel. Compound reactions are a little slower and at lower-energies. They generally involve many collisions with nucleons in the target, leading to collective excitations within the target nucleus. At some intermediate step in the reaction,
Table 4.1: Reaction types (column 1), their general notation and a specific example (column 2), and their defining characteristic as well as some examples of what they can be used to study in the laboratory (column 3).

<table>
<thead>
<tr>
<th>Reaction Type</th>
<th>Notation</th>
<th>Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic Scattering</td>
<td>$A(a,a)A$</td>
<td>$^{208}\text{Pb}(n,n)^{208}\text{Pb}$</td>
</tr>
</tbody>
</table>
|                     | $^{208}\text{Pb}(n,n)^{208}\text{Pb}$ | - internal states unchanged
|                     |                   | - extract effective interactions (optical potentials), interaction radii, density distributions. |
| Inelastic Scattering| $A(a,a')A^*$      | $^{90}\text{Zr}(\alpha,\alpha')^{90}\text{Zr}^*$                          |
|                     |                   | - excitation of target/projectile
|                     |                   | - extract electromagnetic transitions or nuclear deformations                  |
| Charge exchange     | $A(a,c)C$        | $^{14}\text{C}(p,n)^{14}\text{N}$                                             |
|                     | $^{14}\text{C}(p,n)^{14}\text{N}$ | - mass numbers unchanged
|                     |                   | - study beta decays and the weak interaction                                    |
| Capture             | $A(a,\gamma)C$   | $^{16}\text{O}(\alpha,\gamma)^{20}\text{Ne}$                              |
|                     | $^{16}\text{O}(\alpha,\gamma)^{20}\text{Ne}$ | - projectile captured, energy emitted
|                     |                   | - determine resonance energies and widths                                       |
| Breakup             | $d + ^{90}\text{Zr} \rightarrow ^{90}\text{Zr}^* + p + n$ | $^{90}\text{Zr}^*$ \rightarrow $^{90}\text{Zr}^*$ + $p$ + $n$               |
|                     |                   | - projectile breaks apart
|                     |                   | - extract properties of loosely bound states                                    |
| Knockout            | $A(a,a'b)B$      | $^{16}\text{O}(\alpha,2\alpha)^{12}\text{C}$                               |
|                     | $^{16}\text{O}(\alpha,2\alpha)^{12}\text{C}$ | - target emits particles, projectile continues on
|                     |                   | - probe structure of weakly bound nuclei                                        |
| Pickup              | $A(a,c)C$        | $^{90}\text{Zr}(d,p)^{91}\text{Zr}^*$                                       |
|                     | $^{90}\text{Zr}(d,p)^{91}\text{Zr}^*$ | - piece of projectile absorbed by target
|                     |                   | - extract spin, parity and orbital occupancy in valence shells                 |
| Stripping           | $A(a,c)C$        | $^{157}\text{Gd}(^3\text{He},\alpha)^{156}\text{Gd}^*$                      |
|                     | $^{157}\text{Gd}(^3\text{He},\alpha)^{156}\text{Gd}^*$ | - piece of target absorbed by projectile
|                     |                   | - extract spin, parity and orbital occupancy in valence shells                 |
the target and projectile are totally fused and indistinguishable, which means that the exit channel theoretically has no memory of the entrance channel.

In some ways, the distinction between direct and compound reactions is poorly-defined. For example, direct reactions can involve multiple collisions between the projectile and particles within the target, but there is no consensus about exactly how many collisions warrants a shift from treating the reaction as direct to treating it as compound. Reaction mechanisms actually exist on a continuum between purely direct and purely compound. Somewhere in between these two extremes lies resonance reactions, which are a little slower than direct reactions, but faster than compound.

4.2 Nuclear Reaction Observables

Cross sections – typically measured in barns (b) – are a measure of the characteristic area of a system, which quantifies the probability for a reaction to take place: a larger characteristic area is associated with a greater probability for a reaction to take place. A total cross section integrates the angular distribution of flux over all angles, and is the same regardless of whether one is in the laboratory frame or CM frame of the system. The total cross section is denoted \( \sigma(E) \), and is dependent on the energy \( E \) of the incident beam. Cross sections are also often reported for a fixed incident beam energy, as a function of the angles at which the emitted particles are measured. These are called differential cross sections and are written \( d\sigma/d\Omega \) for angle \( \Omega \).

Direct reactions tend to have very forward-peaked differential cross sections, meaning that they are large for very small angles. This follows from the physics: if there is little momentum transfer, then it stands to reason that the emitted particles do not shift far from their incoming trajectory. Compound reactions, on the other hand, tend to have differential cross sections centered on 90°. Resonance reactions are typically understood in terms of their energy-dependent total cross section, rather than an angular distribution. The total cross section of a resonance reaction has sharp peaks centered on resonance energies, as in figure (4.1).
4.2.1 Reaction Rates for Astrophysics

The cross section is important because it is the bridge between theory and experiment. However, what is needed for nuclear astrophysics is actually the reaction rate. The cross section can be used to determine the reaction rate.

Consider a capture reaction \( A(a, \gamma)C \) dominated by a single narrow resonance. The energy-dependent cross section takes a Breit-Wigner form,

\[
\sigma_{BW}(E) = \frac{\pi \hbar^2}{2 \mu E} \frac{2J_r + 1}{(2J_A + 1)(2J_a + 1)} \frac{\Gamma_1 \Gamma_2 \ldots}{(E_r - E) + \Gamma^2/4},
\]

(4.3)

for the reduced mass of the system \( \mu = m_A m_a / (m_A + m_a) \) with \( m_a \) the mass of the projectile \( a \) and \( m_A \) the mass of the target \( A \). The \( J_r, J_A, \) and \( J_a \) are the angular momenta (often referred to as “spin,” but not to be confused with intrinsic spin) of the resonance state in the residual \( C \), the target, and projectile, respectively. The energy \( E \) is the CM
energy of the system, while the energy $E_r$ is the CM resonance energy associated with the $J_r$ resonance. Finally, the total width $\Gamma$ is a sum of all the partial widths $\Gamma_1, \Gamma_2, \ldots$ associated with de-excitation and decay channels. As an example, the Breit-Wigner cross section for the $^{16}\text{O}(\alpha, \gamma)^{20}\text{Ne}$ reaction through the 5.76 MeV $1^-$ state in $^{20}\text{Ne}$ includes only two partial widths: one for decay by $\alpha$ emission, and another for de-excitation through gamma emmission.

In an astrophysical environment, we can assume that the relative energy $E$ of reactant particles $A$ and $a$ has a Maxwell-Boltzmann distribution

\[
f(E) = 2\sqrt{\frac{E}{\pi}} \left(\frac{1}{kT}\right)^{3/2} e^{-E/kT}. \tag{4.4}\]

That is, we assume that the particles are freely moving and have relatively few interactions. Here, $k$ is Boltzmann’s constant and $T$ the temperature.

The thermonuclear reaction rate $\langle \sigma \nu \rangle$ is the product of the cross section and this Boltzmann distribution of the velocity, averaged over all energies

\[
\langle \sigma \nu \rangle = \left(\frac{8}{\pi \mu}\right) \frac{1}{(kT)^{3/2}} \int_0^\infty E\sigma(E)e^{-E/kT} dE. \tag{4.5}\]

Then, for an alpha-capture reaction dominated by a single resonance, the thermonuclear reaction rate is given

\[
\langle \sigma \nu \rangle = \frac{\sqrt{2\pi} h^2}{(\mu kT)^{3/2}} \frac{2J_r + 1}{(2J_A + 1)(2J_a + 1)} \int_0^\infty \frac{\Gamma_\alpha \Gamma_\gamma}{(E_r - E)^2 + \Gamma^2/4} e^{-E/kT} dE, \tag{4.6}\]

where $\Gamma_\alpha$ is the alpha partial width and $\Gamma_\gamma$ is the width of the de-excitation through gamma emmission.

At this point, an approximation is made: for sufficiently narrow resonances, the partial widths and $e^{-E/kT}$ are approximately constant, and can be approximated with their values at $E_r$. So, the lower limit of the integral here is taken to be $-\infty$, and the reaction rate
reduces to
\[
\langle \sigma \nu \rangle_r = \left( \frac{2\pi}{\mu kT} \right)^{3/2} h^2 \frac{2J_r + 1}{(2J_A + 1)(2J_a + 1)} \frac{\Gamma_\alpha \Gamma_\gamma}{\Gamma} e^{-E_r/k_r T}.
\]  

The following expression is typically used to compute astrophysical nuclear reaction rates in units of cm\(^3\)/s/mole, and reduces Eq. (4.7) by simplifying constants and multiplying through by Avogadro’s Number \(N_A\):
\[
N_A \langle \sigma \nu \rangle_r = 1.5399 \times 10^{11} \left( \frac{\mu T_9}{9} \right)^{3/2} e^{-11.605E_r/T_9} (\omega \gamma)_r,
\] (4.8)

where the resonance strength \( (\omega \gamma)_r \) is given by
\[
(\omega \gamma)_r = \frac{2J_r + 1}{(2J_A + 1)(2J_a + 1)} \frac{\Gamma_\alpha \Gamma_\gamma}{\Gamma}.
\] (4.9)

In Eqs. (5.19) and (4.9), temperatures \(T_9\) are given in GK, the resonance energy \(E_r\) in MeV, the reduced mass in MeV/c\(^2\), and the widths in MeV.

### 4.2.2 Alpha partial Widths and ANCs

To compute the astrophysical reaction rate for an alpha-capture reaction, then, one must determine (1) the resonance energy \(E_r\), (2) the alpha partial width \(\Gamma_\alpha\), and (3) the gamma branching ratio \(\Gamma_\gamma/\Gamma\). The resonance energy and branching ratio can both be measured directly through studying capture reactions. One can also measure the total resonance strength [as in Eq. (4.9)] in a direct capture reaction. The alpha partial width, however, can only be extracted from experimental data through model-dependent means; specifically, through the use of DWBA calculations that require alpha OMPs. As an alternative, one can determine the alpha partial width within a theoretical framework.

**Resonances** – The partial width of a resonance state corresponding to the emission of an
\(a\)-particle cluster with relative angular momentum \(l\) is given by \([187,188]\)

\[
\Gamma_a(r_c) = 2P_l(r_c) \frac{\hbar}{2\mu r_c} \left[ru_{\nu l\ell}(r)\right]_{r=r_c}^2,
\]

(4.10)

where \(P_l(r)\) is the Coulomb penetrability, and \(ru_{\nu l\ell}(r)\rfloor_{r=r_c}\) is the spectroscopic amplitude (sometimes called the “formation amplitude” such as in Ref. [187]) at a separation distance \(r = r_c\) between the centers of mass of the \(a\)-particle cluster and the \((A - a)\)-particle cluster. This is an \(R\)-matrix equation, with a channel radius \(r_c\), where the interior nuclear wave function and exterior, Coulomb-dominated wave function, are matched. The partial width can also be written

\[
\Gamma_a(r_c) = 2P_l(r_c) \gamma_{\nu l}^2(r_c),
\]

(4.11)

that is: a product of the penetrability, which is driven by the Coulomb force at large distances, and the quantity \(\gamma_{\nu l}^2(r_c) = \frac{\hbar}{2\mu r_c} \left[ru_{\nu l\ell}(r)\right]_{r=r_c}^2\), also called the reduced width, which contains information about the wave function at small distances (it is “reduced” through the exclusion of the penetrability). The norm of the spectroscopic amplitude,

\[
\int_0^\infty |ru_{\nu l\ell}(r)|^2 \, dr,
\]

(4.12)

is the spectroscopic factor.

The spectroscopic amplitude is defined for total angular momentum and parity, \(J^\pi\), and angular momentum \(I\) for the clusters in channel \(\nu\). For a two-cluster system, the channel is defined by the spin and parity of each of the clusters, \(\nu = \{\alpha, \alpha', I^\pi', \alpha'', I''^\pi\}\). The labels \(\alpha, \alpha'\) and \(\alpha''\) denote all other quantum numbers needed to fully characterize their respective states.

The Coulomb penetrability \(P_l(r)\) is determined by \(H_l^+(\eta, kr)\), the outgoing spherical Hankel function solution to the Coulomb equation defined by the Sommerfeld parameter.
\[ \eta = \frac{Z_{A-a}Z_a\mu e^2}{\hbar k} \] for two clusters of charge \(Z_{A-a}\) and \(Z_a\),

\[ P_l(r) = \frac{kr}{|H^+_l(\eta, kr)|^2}, \quad (4.13) \]

where the momentum \(k\) corresponds to the energy of the emitted \(a\)-particle cluster \(E = \frac{\hbar^2 k^2}{2\mu}\).

**Bound States** – For bound states, the external wave function is not given by an oscillatory Coulomb-Hankel function, but rather by an asymptotically-decaying Whittaker function:

\[ W_{-\eta_B,l+\frac{1}{2}}(2\kappa_B r) \xrightarrow{x \to \infty} (2\kappa_B r)^{-\eta_B e^{-\kappa_B r}}. \quad (4.14) \]

Here, \(\kappa_B = \sqrt{-2\mu E}/\hbar\), for a negative energy \(E\), and \(\eta_B = \frac{Z_{A-a}Z_a\mu e^2}{\hbar^2 \kappa_B}\) is the associated Sommerfeld parameter. The observable ANC \(C_l\) determines the amplitude of the exterior wave function at large distances \(r\), so that the exterior bound state wave function is written \[ \phi_{J\pi,ext}^{J\pi}(r) = C_{J\pi}W_{-\eta_B,l+\frac{1}{2}}(2\kappa_B r). \quad (4.15) \]

The ANC can be determined through matching the exterior wave function with the interior bound state wave function,

\[ \phi_{J\pi,int}^{J\pi}(r) = Aru_{J\pi}^{J\pi}(r), \quad (4.16) \]

where \(A\) is the norm of the interior wave function. Since the complete (interior + exterior) wave function must be normalized to unity, the norm of the interior contribution is given

\[ A^2 = 1 - (C_{J\pi})^2 \int_{r_c}^{\infty} |W_{-\eta_B,l+\frac{1}{2}}(2\kappa_B r)|^2 dr. \quad (4.17) \]

Matching the interior and exterior solutions at the channel radius \(r_c\) yields the following
expression for the ANC:

\[
(C^{J_\nu}_{\nu,II})^2 = \frac{|ru^{J_\nu}_{\nu,II}(r)|^2}{\left|W_{-\eta B,l+\frac{3}{2}}(2\kappa_B r)\right|^2 r_c + \left|ru^{J_\nu}_{\nu,II}(r)\right|^2 r_c \int_{r_c}^{\infty} \left|W_{-\eta B,l+\frac{3}{2}}(2\kappa_B r)\right|^2 dr}.
\] (4.18)
5 A New Many-Body Method for Nuclear Reactions

This chapter outlines the main focus of the work of this dissertation: the development of a new many-body theory for nuclear reactions, and its application to the $^{20}\text{Ne}$ system. Sections 1 and 2 comprise the derivation of the theory, and are supplemented by the appendices. The following sections present calculations of the ground state wave function of $^{20}\text{Ne}$ as a $\alpha + ^{16}\text{O}$ cluster system and its associated ANC, the spectroscopic amplitude and alpha partial width of the 1.06 MeV $1^-$ resonance state, the contribution through the 1.06 MeV $1^-$ resonance to the $^{16}\text{O}(\alpha, \gamma)^{20}\text{Ne}$ reaction rate, and the impact on XRB abundances produced in a simulation using this theoretical rate. The work presented in this chapter is in preparation for publication [189].

5.1 Coordinates

For a system of $A$ particles, the set of laboratory coordinates is denoted $\vec{r}_1, \ldots, \vec{r}_A$. A two-cluster system, with an $(A-a)$-particle cluster and an $a$-particle cluster separated by $\vec{r}_{A-a,a}$, can be divided into two distinct sets of lab coordinates, $\vec{r}_1, \ldots, \vec{r}_{A-a}$ and $\vec{r}_{A-a+1}, \ldots, \vec{r}_A$ (see Fig. 5.1). The centers of mass of the two clusters ($\vec{R}'$ and $\vec{R}''$) and the composite system $\vec{R}$ are related:

\[
\vec{R}' = \frac{1}{A-a} \sum_{i=1}^{A-a} \vec{r}_i \tag{5.1}
\]

\[
\vec{R}'' = \frac{1}{a} \sum_{i=A-a+1}^{A} \vec{r}_i \tag{5.2}
\]

\[
\vec{R} = \frac{1}{A} \sum_{i=1}^{A} \vec{r}_i = \frac{(A-a)\vec{R}' + a\vec{R}''}{A} \tag{5.3}
\]

\[
\vec{r}_{A-a,a} = \vec{R}'' - \vec{R}'. \tag{5.4}
\]

We define a set of coordinates relative to $\vec{R}$,

\[
\vec{\zeta}_i = \vec{r}_i - \vec{R}. \tag{5.5}
\]
Figure 5.1: An illustration of the coordinates used in the formalism. The $\vec{r}_i$ are the independent particle coordinates in the laboratory frame. The centers of mass of the individual clusters are given by $\vec{R}'$ and $\vec{R}''$, while the total system CM is $\vec{R}$. The relative separation of the clusters is $\vec{r}_{(A-a),a}$. The coordinates used in this formalism are the $\vec{\zeta}_i$ coordinates, given relative to $\vec{R}$.

The two clusters can be written in terms of coordinates $\vec{\zeta}' \equiv \vec{\zeta}_1, \ldots, \vec{\zeta}_{A-a}$ and $\vec{\zeta}'' \equiv \vec{\zeta}_{A-a+1}, \ldots, \vec{\zeta}_A$, respectively. Note, from Eq.(5.1) and from Eq.(5.5) that $\sum_{i=1}^{A} \vec{\zeta}_i = 0$, so that there are only $A - 1$ independent relative coordinates. The translationally invariant two-cluster system is fully described by the relative coordinates

$$\vec{\zeta} = \{\vec{\zeta}_1, \ldots, \vec{\zeta}_{A-a}, \vec{\zeta}_{A-a+1}, \ldots, \vec{\zeta}_{A-1}\}. \quad (5.6)$$

5.2 Determining Partial Widths and ANCs Within a Many-Body Framework

Determining either the resonance partial width or the ANC of a bound state requires a calculation of the spectroscopic amplitude. The spectroscopic amplitude is given through an overlap between the composite $A$-particle state $\Psi_A$ and the cluster state. For the partition into $a$- and $(A-a)$-particle clusters, with interior wave functions $\psi_{(a)}$ and $\psi_{(A-a)}$, the spectroscopic amplitude $ru^J_{\nu I I}(r)$ is given by [187]

$$u^J_{\nu I I}(r) = \sum_{M_{1m}} C^J_{I M_{1m}} \int d\hat{r} Y^*_{\nu m}(\hat{r}) u^I_M(\hat{r}), \quad (5.7)$$
\[ u^{JM_l}_\nu (\vec{r}) = \int d^3 \vec{\zeta} \left[ \Psi_{(A)}^{\alpha J^\pi M} (\vec{\zeta}) \right] \times A [\{ \psi_{(A-a)}^{\alpha' J^\pi' M'} (\vec{\zeta}') \times \psi_{(a)}^{\alpha'' J^\pi'' M''} (\vec{\zeta}'') \}]^{JM_l} \delta (\vec{r} - \vec{r}_{A-a,a}). \]

The delta function is expanded in HO functions with the reduced HO constant \( b_{\text{rel}} = \sqrt{\hbar/\mu \Omega} \) [using a reduced mass as defined for Eq. (4.3)]

\[ \delta (\vec{r} - \vec{r}_{A-a,a}) = \sum_{n l' m'} R_{nl'} (r) Y_{l'm'} (\hat{\vec{r}}) R_{nl'} (r_{A-a,a}) Y_{l'm'} (\hat{\vec{r}}_{A-a,a}). \]  

(5.8)

We define \( R_{nl}(r_{A-a,a}) \) as the relative wave function, and introduce \( \int \phi^\dagger_{000}(\vec{R}) \phi_{000}(\vec{R}) d^3 \vec{R} = 1 \) for HO basis state functions \( \phi_{nlm}(\vec{R}) \) with primary quantum number \( n = 0 \), so that \( l = 0 \) and \( m = 0 \). The spectroscopic amplitude of Eq. (5.7) is now written in terms of the composite \( A \)-particle wave function with an explicitly separable center-of-mass contribution \( \phi_{000}(\vec{R}) \), and a cluster basis wave function with the same center-of-mass motion,

\[ u^{J^\pi T}_{\nu l l'} (r) = \sum_n R_{nl}(r) \int d^3 \vec{\zeta} d^3 \vec{R} \left[ \Psi_{(A)}^{\alpha J^\pi M} (\vec{\zeta}) \phi_{000}(\vec{R}) \right]^\dagger \times A [\{ \psi_{(A-a)}^{\alpha' J^\pi' M'} (\vec{\zeta}') \times \psi_{(a)}^{\alpha'' J^\pi'' M''} (\vec{\zeta}'') \}]^I \times \chi_{nl}(\vec{r}_{A-a,a}, \phi_{000}(\vec{R})) J^\pi M, \]  

(5.9)

where the cluster basis wave function is a product of intrinsic wave functions for each of the clusters coupled to the relative motion wave function \( \chi_{nlm}(\vec{r}_{A-a,a}) \). Or, equivalently,

\[ u^{J^\pi}_{\nu l l'} (r) = \sum_n R_{nl}(r) \langle (A) \alpha J^\pi M | (\alpha' I^\pi', \alpha'' I^\pi'') I, nl; J^\pi M \rangle, \]  

(5.10)

which is independent of \( M \). To calculate the overlap in Eq. (5.10), we use a many-particle state for the composite system \( A \), calculated in the symmetry-adapted basis. For the symmetry-adapted basis, the additional quantum numbers \( \alpha' = \bar{\alpha}' \omega' \kappa'(L'S') \) and \( \alpha'' = \bar{\alpha}'' \omega'' \kappa''(L''S'') \), where \( \omega' = N'_\omega (\lambda'_\omega \mu'_\omega) \) (likewise for \( \omega'' \)) are the quantum numbers defining
total excitations and deformation \cite{157}, \( \kappa \) is a multiplicity in angular momentum \( L \) for a given \((\lambda \mu)\), and \( S \) denotes intrinsic spin. Similarly the relative motion \( |nl| \) becomes \( |n(n_0)l| \).

The composite wave function of Eq. \((5.10)\) is expanded in the symplectic basis for a single symplectic irrep with \( \alpha = \bar{\alpha}\sigma_0(L_0S) \):

\[
| (A)\bar{\alpha}\sigma_0(L_0S)J^\pi M \rangle = \sum_{\bar{n}_0\rho_0\omega_0\kappa_0} c_{\bar{n}_0\rho_0\omega_0\kappa_0} | (A)\bar{\alpha}\sigma_0\bar{n}_0\rho_0\omega_0\kappa_0(L_0S)J^\pi M \rangle, \tag{5.11}
\]

where the symplectic state and its quantum numbers are defined in Eqs. \(3.2\) and \(3.3\).

Note that, through the transformation into the symplectic basis, the channel is now identified by

\[
\nu = \{ \bar{\alpha}\sigma_0S; \bar{\alpha}'\omega'\kappa'L'S'I''\pi''; \bar{\alpha}''\omega''\kappa''L''S''I''\pi'' \}. \tag{5.12}
\]

That is, a single channel is given by a single symplectic irrep \( |\sigma_0S \rangle \) of the composite system, and two clusters that are each fixed in some state given by its deformation and spin.

This is generalizable to a number of symplectic irreps, however, typically a single symplectic irrep accounts for a significant portion of the wave function, often as much as \(70 - 80\%\) \cite{122}. The wave function for the composite system can be computed using any many-body formalism, as long as it is ultimately expanded in symplectic basis states \( |(A)\bar{\alpha}\sigma_0\bar{n}_0\rho_0\omega_0\kappa_0L_0M_0 \rangle \), coupled with spin to the proper total angular momentum \( J^\pi \).

Through recoupling to good angular momentum \( L \) and spin \( S \), and then to the SU(3) basis, the expression for the spectroscopic amplitude in Eq. \((5.10)\) can be rewritten:
\[ w_{\nu_{II}}^{LM}(r) = \sum_n R_{nl}(r) \sum_{\rho L_{\kappa}} \Pi_{LS'I'I} \left\{ \begin{array}{ccc} L' & S' & I' \\ L'' & S'' & I'' \\ L & S & I \end{array} \right\} \langle \omega' \kappa' L'; \omega'' \kappa'' L'' \| \omega \kappa L \rangle_{\rho} \]

\times \sum_{\rho_0 \omega_0 \kappa_0 L_0} \Pi_{L_0} \left\{ \begin{array}{ccc} S & L & I \\ l & J & L_0 \end{array} \right\} (-)^{l+I+L_0+S} \langle \omega \kappa L; \omega_0 \kappa_0 L_0 \| (n0)l \rangle_{\rho_0} \rho_0 \omega_0 \kappa_0 L_0 \rangle_{\rho_0} \]

\times \sum_{\bar{n}_0} c_{\bar{n}_0 \rho_0 \omega_0 \kappa_0 L_0} \langle (A) \bar{\alpha} \sigma_0 \bar{n}_0 \rho_0 \omega_0 \Omega_0 \| (\alpha \omega; (n0)) \rangle_{\rho_0} \rho_0 \omega_0 \Omega_0 \). (5.13)

Where we introduce the notation \( \Omega = \kappa L M_L \). The symbol \( \Pi_X = \sqrt{2X + 1} \) is the dimension of the SU(2) quantum number \( X \), and the double-bar coefficients,

\[ \langle \omega' \kappa' L'; \omega'' \kappa'' L'' \| \omega \kappa L \rangle_{\rho} \) and \( \langle \omega \kappa L; \omega_0 \kappa_0 L_0 \| (n0)l \rangle_{\rho_0} \rho_0 \omega_0 \kappa_0 L_0 \rangle_{\rho_0} \],

are SU(3) Clebsch-Gordan coefficients that are SU(2)-reduced. For a general SU(3) Clebsch-Gordan coefficient, that reduction is [171]

\[ \langle \omega' \kappa' L'M'; \omega'' \kappa'' L''M'' \| \omega \kappa L M \rangle = \sum_{\rho} C_{L'M'LM''M''}^{LM} \langle \omega' \kappa' L'; \omega'' \kappa'' L'' \| \omega \kappa L \rangle_{\rho}. \] (5.14)

The cluster basis wave function in spatial coordinates, with \( \alpha = (\alpha', \alpha'') \rho \), is

\[ |(\alpha \omega; (n0)) \rangle_{\rho_0 \omega_0 \Omega_0} = \{|\alpha'\rangle \times |\alpha''\rangle\}^{\rho \omega \times (n0)}|\rangle_{\rho_0 \omega_0 \Omega_0}. \] (5.15)

The spectroscopic amplitude of Eq. (5.13) depends on the overlap

\[ \langle (A) \bar{\alpha} \sigma_0 \bar{n}_0 \rho_0 \omega_0 \Omega_0 \| (\alpha \omega; (n0)) \rangle_{\rho_0 \omega_0 \Omega_0} \].
which we aim to derive and calculate within a microscopic framework, as described next.

With the assumption that each of the two clusters is fixed to the bandhead of a symplectic irrep, this overlap is calculated as [94,95]:

\[
\sum_{n_0} (-)^{\bar{\omega}_0 - \omega_0} U[\sigma_0 n_0 \bar{\omega}_0 (0 2); \omega_0 \rho_0 1; \bar{n}_0 \bar{\rho}_0] (\bar{n}_0 || \mathcal{B}^{(02)} || n_0) | \Delta \Omega_K (n_0 \omega_0, \bar{n}_0 \bar{\omega}_0) \rangle^{1/2} \\
\times \langle \bar{\alpha} \sigma_0 n_0 \rho_0 \omega_0 \Omega_0 | (\omega; n(n0)) \rho_0 \omega_0 \Omega_0 \rangle \cdot \sqrt{\text{dim}(n0) U[\omega(n0) \bar{\omega}_0 (0 2); \omega_0 \rho_0 1; (n-2) 0 \bar{\rho}_0]}
\times \langle (A) \bar{\alpha} \sigma_0 \bar{n}_0 \bar{\rho}_0 \bar{\omega}_0 \bar{\Omega}_0 | (\omega; n-2(n-2) 0) \bar{\rho}_0 \bar{\omega}_0 \bar{\Omega}_0 \rangle,
\] (5.16)

where \( N_{n_0} = N_{\bar{n}_0} + 2 \). The \( \mathcal{B}^{(02)} \) is the symplectic lowering operator [defined in Eq. (3.4)], the \( U \) symbol is an SU(3) \( U \)-Racah coefficient, and \( \text{dim}(n0) \) is the SU(3) dimension of \( (n0) \) [171]. Although we maintain the notation, it should be noted that the overlap is independent of \( \Omega_0 \) and \( \bar{\Omega}_0 \).

The overlap at \( N_{n_0} = 0 \) between the bandhead of the symplectic irrep describing the composite system and the cluster configuration with the lowest energy relative motion is always 1, and is used as the base case for the recursion. The antisymmetrization is included in the overlap through the antisymmetrization of the base case. Because the antisymmetrizer depends only on \( A - a \) and \( a \), it is the same for each \( n \), so the antisymmetrization of Eq. (5.9) propagates down to the base case.

The formula in Eq. (5.16) is valid for all \( \rho_0 \omega_0 \), given \( n_0 \), but becomes a simple recursive formula for specific states of interest, for which there is a single \( \omega_0 \) (with \( \rho_0 = 1 \)) for each \( n_0 \).

The symplectic states are normalized through the use of the \( \mathcal{K} \)-matrix [156, 190, 191]. Although the \( \mathcal{K} \)-matrix is not typically diagonal, in the limit of large \( \sigma_0 \), it reduces to the diagonal case. We adopt the notation

\[
\Delta \Omega_K (n_0 \omega_0, n'_0 \omega'_0) = \Omega_K (n_0 \omega_0) - \Omega_K (n'_0 \omega'_0),
\] (5.17)
with $K$-matrix coefficients $\Omega_K(n\omega)$ given by [156]

$$
\Omega_K(n\omega) = \frac{1}{4} \sum_{j=1}^{3} \left[ 2\omega_j^2 - n_j^2 + 8(w_j - n_j) - 2j(2w_j - n_j) \right],
$$

(5.18)

where $j$ denotes the three spatial coordinates, with $n_1 = \frac{N_n + 2\lambda_n + \mu_n}{3}$, $n_2 = \frac{N_n - \lambda_n + \mu_n}{3}$, and $\frac{N_n - 2\lambda_n - 2\mu_n}{3}$ (the $\omega_j$ are similarly defined for $N_\omega, \lambda_\omega, \mu_\omega$). The cluster basis is normalized by Hecht in Ref. [192]. The normalization is derived for cluster systems comprised of an $\alpha$ particle and a heavy fragment, with total particle number $12 \leq A \leq 24$.

### 5.3 Results

The formalism is validated in $^{20}$Ne, which is a well-known cluster system. In particular, the excited $1^-$ state at 5.79 MeV above the ground state (or 1.06 MeV above the $\alpha + ^{16}$O threshold in the center-of-mass frame\(^1\)), is understood to be a purely $\alpha$-cluster state. Although alpha partial widths are not generally directly measurable in experiment because of very low cross-sections at astrophysically relevant energies, the natural width of the $^{20}$Ne $1^-$ state is known to be 28(3) eV. There is a nearby $3^-$ state at 5.62 MeV above the ground state (0.89 MeV above the $\alpha + ^{16}$O threshold) that should typically be treated in a coupled-channels framework with the $1^-$ state. However, both states are very narrow, especially the $3^-$ state, and, as their coupling is negligible, they can be treated in separate single-channel calculations. Calculations for the $3^-$ state are neglected in the current study.

In all calculations shown here, we take the experimental resonance energy (1.06 MeV for the $1^-$ resonance), or the experimental energy for the bound states. A self-consistent calculation of the energy requires a number of large-scale calculations of all three systems – the composite system, the $A-a$ cluster, and the $a$ cluster – to determine converged thresholds and energy differences for each of the two clusters, which is outside the scope of this work.

\(^1\)For a two-cluster system, its energy in the center-of-mass frame $E_{CM}$ is related to the projectile laboratory-frame energy $E_{lab}$ as $E_{lab} = (\frac{m_1 + m_2}{m_2})E_{CM}$, where $m_1$ is the mass of the projectile and $m_2$ is the mass of the target.
5.3.1 Resonance Spectroscopic Amplitudes and Bound State Wave Functions

In this study, the composite wave function is calculated using two many-body frameworks: (1) the microscopic NCSpM [109], and (2) the \textit{ab initio} SA-NCSM [157]. Both models have yielded energy spectra and observables (radii, quadrupole moments, and $E2$ transitions) in close agreement with experiment (see Chapter 3 and Refs. [109,118,157]).

The NCSpM uses the symplectic Sp$(3,R)$ basis and a microscopic Hamiltonian defined in Eq. (3.13). Wave functions are calculated in the basis of a single symplectic irrep, including all excitations above the lowest-energy configuration up to the truncation parameter $N_{\text{max}}$ [109,110,118]. The SA-NCSM is a no-core shell model that is capable of implementing realistic $NN$ interactions within either the SU$(3)$ symmetry-adapted basis (SA-NCSM/SU$(3)$) [157] or the Sp$(3,R)$ symmetry-adapted basis (SA-NCSM/Sp$(3,R)$) [123]. For the SA-NCSM/SU$(3)$, we make the approximation that a given SU$(3)$ basis state belongs to only a single symplectic irrep, ignoring the mixing of symplectic irreps within a given SU$(3)$ state.
All wave functions are renormalized to a selected model space consisting of the stretched-coupled states of the leading irrep, which are the most deformed states in the irrep [i.e., \((\lambda_n \mu_n) = (N_n, 0)\) and \((\lambda_\omega \mu_\omega) = (\lambda_\sigma + N_n, \mu_\sigma)\)], and the next-most deformed states in the irrep [i.e., \((\lambda_n \mu_n) = (N_n - 4, 2)\) and \((\lambda_\omega \mu_\omega) = (\lambda_\sigma + N_n - 4, \mu_\sigma + 2)\)]. Note that, for the \(^{20}\text{Ne}\) gs in the SA-NCSM/SU(3) model with \(N_{\text{max}} = 8\) and \(\hbar \Omega = 15\) MeV, 70\% of the wave function is described with just the leading \(\sigma = 48.5(8.0)\) irrep \([123]\). By down-selecting to include only the most deformed and second most-deformed contributions, we retain 99\% of that irrep.

We compute the bound state wave function [see Eq. (4.15) and (4.16)] within this framework for the \(^{20}\text{Ne}\) gs (Fig. 5.2). The relative motion wave function of \(^{16}\text{O} + \alpha\) in the gs of the composite \(^{20}\text{Ne}\) nucleus determined using an SA-NCSM/SU(3) calculation (blue) is nearly indistinguishable from the SA-NCSM/Sp(3, \(\mathbb{R}\)) calculation (red), for the same \(\hbar \Omega = 15\) MeV. This implies that the predominant contribution to a single SU(3) state is indeed coming from the leading symplectic irrep, and so the assumption used in the SA-NCSM/SU(3) calculations is reasonable. To guide the eye, we compare to the NCSpM wave function (Fig. 5.2, grey curve), calculated with \(N_{\text{max}} = 22\), \(\hbar \Omega = 15\) MeV. The result is very similar to the SA-NCSM calculations, implying that the wave functions are reasonable.

In a similar fashion, Fig. 5.3(a) compares the spectroscopic amplitudes (not the bound state wave functions) for the 1\(^{-}\) resonance of the \(\alpha + ^{16}\text{O} \rightarrow ^{20}\text{Ne}\) cluster system. The \(^{20}\text{Ne} 1\(^{-}\) wave function is calculated in the SA-NCSM/Sp(3, \(\mathbb{R}\)) (red) and SA-NCSM/SU(3) (blue) with \(N_{\text{max}} = 5\) and \(\hbar \Omega = 15\) MeV. Again, all wave functions are renormalized within the leading \(\sigma = 49.5(9.0)\) irrep, and the close agreement between the SA-NCSM/SU(3) and SA-NCSM/Sp(3, \(\mathbb{R}\)) spectroscopic amplitudes indicates that the assumption used in the SA-NCSM/SU(3) calculations is reasonable.

It is interesting to note that, because the 1\(^{-}\) state in \(^{20}\text{Ne}\) is a resonance, the wave function is not expected to decay in the asymptotic regime as it does in the gs case; rather, the exterior resonance wave function has oscillatory behavior due to the influence of the
Figure 5.3: Spectroscopic amplitudes for the 1.06 MeV 1− resonance in the α + 16O → 20Ne system. All 20Ne wave functions are renormalized within the selected σ = 49.5(9.0) irrep. Interior and exterior components are shown with solid and dashed lines, respectively, except where otherwise indicated. (a) The 20Ne wave functions are calculated using the SA-NCSM/SU(3) (blue) and SA-NCSM/Sp(3, R) (red) with N_{max} = 5, \hbar\Omega = 15 MeV. The inset shows the asymptotic oscillatory behavior of the wave functions for the SA-NCSM/Sp(3, R) case. The dotted red line shows the form of the SA-NCSM/Sp(3, R) spectroscopic amplitude without matching in the asymptotic regime to the Coulomb-Hankel functions. (b) The 20Ne wave functions are calculated using the SA-NCSM/SU(3) with N_{max} = 9, \hbar\Omega = 13 (blue), N_{max} = 9, \hbar\Omega = 15 MeV (grey), N_{max} = 7, \hbar\Omega = 15 MeV (black), N_{max} = 7, \hbar\Omega = 17 MeV (red), and NCSpM with N_{max} = 23, \hbar\Omega = 15 MeV (green – interior dashed, exterior dotted) Coulomb interaction, as shown for the SA-NCSM/Sp(3, R) in the inset in Fig. 5.3(a). In this exterior regime, the form of the spectroscopic amplitude is driven by the spherical Coulomb-Hankel functions H^{+}_{l}(\eta, kr). Without matching to the Coulomb-Hankel functions in the exterior region, the form of the spectroscopic amplitude is significantly changed (see 5.3(a), red dotted curve). Having the correct asymptotic oscillatory behavior, therefore, is of integral importance to determining spectroscopic factors [i.e., using Eq. (4.12)].

Fig. 5.3(b) shows the spectroscopic amplitudes for the 1− resonance of α + 16O → 20Ne calculated with the SA-NCSM/SU(3) 1− wave functions for three values of \hbar\Omega. It is clear that the spectroscopic amplitudes depend on \hbar\Omega, but the deviations are not large. In Fig. 5.3(b), we include the N_{max} = 7 (grey) and N_{max} = 9 (black) results for \hbar\Omega = 15 MeV, which are nearly indistinguishable. To guide the eye, we again include the α + 16O → 20Ne spectroscopic amplitude computed using a NCSpM 1− wave function with N_{max} = 23 and \hbar\Omega = 15 MeV (Fig. 5.3(b), green dashed/dotted line). The peak for the NCSpM spectroscopic amplitude
is of a similar magnitude to the SA-NCSM/SU(3) $\hbar \Omega = 15$ MeV result, but the peak occurs for a larger channel radius.

### 5.3.2 ANCs and $\alpha$ Partial Widths

The alpha partial widths $\Gamma_\alpha$ are determined using $^{20}\text{Ne}$ $1^-$ wave functions calculated with the SA-NCSM/SU(3) for a series of increasingly larger model spaces in Fig. 5.4. Calculations are done using an empirical estimate of the HO separation energy, $\hbar \Omega \approx 41/A^{1/3} = 15$ MeV (see Ref. [161]), and two nearby values, $\hbar \Omega = 13, 17$ MeV. We compute the alpha width as a function of the channel radius $r_c$, and report results for the maximum value of the alpha width $\Gamma_\alpha$, where the results are least sensitive to changes in the channel radius, as discussed in Ref. [149]. It should be noted that, in order to compare directly to experiment, one may need to introduce an additional factor, involving the energy-derivative of the shift function (see discussions of “observed” compared to “calculated” widths and reduced widths in Refs. [75, 193] for more information). Previous work has shown that the introduction of this factor slightly reduces the calculated width [75], so reporting the maximum width here gives a close upper bound on the observed width, which could be directly compared to experiment.

The dependence on the $\hbar \Omega$ model space parameter can be understood as a result of the choice to select a single channel radius for which the width is maximum. In making this choice, there is an effective renormalization within the channel radius, and so we cannot expect results to be independent of $\hbar \Omega$. Given the clear convergence with respect to the $N_{\text{max}}$ model space, and the uncertainty introduced by $\hbar \Omega$ seen in Fig. 5.4 we use a linear extrapolation of the $\hbar \Omega = 13$ MeV and $\hbar \Omega = 17$ MeV results to determine an extrapolated alpha partial width of $\Gamma = 8(2) \text{ eV}$, where the error bar is given by the $\sim 13\%$ variation in $\hbar \Omega$ values. Although this result is lower than the alpha partial width of the $1^-$ state in $^{20}\text{Ne}$, $\Gamma_\alpha = 28(3) \text{ eV}$ [194], it should be noted that reproducing the order of magnitude of

\[ \text{The alpha partial width reported here is actually the total width, but the total width and partial width are essentially the same for this resonance [66].} \]
Figure 5.4: Alpha partial widths for the $^{20}\text{Ne}$ $1^-$ resonance, calculated with the SA-NCSM/SU(3) (circles) for three values of $\hbar\Omega$: $\hbar\Omega = 13$ MeV (red), $\hbar\Omega = 15$ MeV (blue), and $\hbar\Omega = 17$ MeV (grey). The NCSpM partial width with $N_{\text{max}} = 22$, $\hbar\Omega = 15$ MeV is also shown (blue square). A linear extrapolation of the $\hbar\Omega = 13$ MeV and $\hbar\Omega = 17$ MeV results is used to determine an extrapolated alpha partial width of $\Gamma = 8(2)$ eV. The error is given by the $\sim 13\%$ variation in $\hbar\Omega$.

$\Gamma_\alpha$ poses a significant challenge to theoretical approaches.

Additionally, further study into the dependence on the parameters $\hbar\Omega$ and $N_{\text{max}}$, and the calculation of the theoretical error bar that results from these dependences is in progress. The NCSpM $\Gamma_\alpha$ result gives us some indication that the SA-NCSM/SU(3) $\hbar\Omega = 15$ MeV $\Gamma_\alpha$ is not fully converged with respect to $N_{\text{max}}$, despite the close agreement between the $\hbar\Omega = 15$ MeV, $N_{\text{max}} = 7$ and $N_{\text{max}} = 9$ SA-NCSM/SU(3) spectroscopic amplitudes.

The ANC is extracted using Eq. (4.18). We compute ANCs as a function of the channel radius $r_c$, with the interior function $r u_{r}^{\gamma} \ell_j (r)$ renormalized to 1 within $r_c$, and report results for the maximum value of the ANC, where the result is least sensitive to changes in the channel radius. The maximum value of the ANC calculated using $^{20}\text{Ne} 0^+_{gs}$ wave functions calculated in an $N_{\text{max}} = 8$, $\hbar\Omega = 15$ MeV model space for the SA-NCSM/SU(3) is $C_{\ell}^{\text{SU}(3), gs} = 2.01 \times 10^8 \text{ fm}^{-1/2}$, and $C_{\ell}^{\text{Sp}(3,R), gs} = 2.09 \times 10^8 \text{ fm}^{-1/2}$ for the SA-NCSM/Sp(3, $R$) in the same model space. The maximum value of the ANC calculated using the NCSpM in an $N_{\text{max}} = 22$ model space is slightly larger: $C_{\ell}^{\text{NCSpM}, gs} = 2.43 \times 10^8 \text{ fm}^{-1/2}$. The $gs$ ANCs are converged with respect to the model space truncation parameter $N_{\text{max}}$ for a given $\hbar\Omega$, as seen in Fig.
5.5. Again, using a linear extrapolation of the $\hbar \Omega = 13$ MeV and $\hbar \Omega = 17$ MeV results, we can determine an extrapolated ANC of $C_l^{\text{SA-NCSM, gs}} = 2.1(3) \times 10^8$ fm$^{-1/2}$, where the error is determined by the $\sim 13\%$ variation in $\hbar \Omega$. Note that ANCs can range from on the order of tenths of fm$^{-1/2}$ for single-particle capture on light systems [195] to, e.g., $10^{14}$ fm$^{-1/2}$ for the 1$^-$ state in $^{16}$O [65, 196]. The ANC is not highly dependent on the energy: a change of $\pm 1$ MeV in the $\alpha + ^{16}$O threshold energy results in a change of less than 10% in the ANC. In order to determine an ANC, then, it is necessary to use a model that properly accounts for the clustering inherent in the system.

In addition to the gs ANC, we compute the ANC for the excited 4.25 MeV 4$^+$ state in $^{20}$Ne, which is just 0.48 MeV below the $\alpha + ^{16}$O threshold. Using an SA-NCSM/SU(3) wave function in $N_{\text{max}} = 8$, with $\hbar \Omega = 15$ MeV, the ANC for the 4$^+$ state is $C_l^{\text{SA-NCSM, 4}^+} = 4.62 \times 10^6$ fm$^{-1/2}$. Near-threshold ANCs, such as this, can be used to determine alpha widths that cannot otherwise be directly measured [66].

Figure 5.5: The $C_l$ in (fm$^{-1/2}$) are calculated for SA-NCSM/SU3 (circles) as a function of the model space truncation parameter $N_{\text{max}}$, and shown for $\hbar \Omega = 13$ MeV (red), $\hbar \Omega = 15$ MeV (blue), and $\hbar \Omega = 17$ MeV (grey) MeV. The NCSpM result with $N_{\text{max}} = 22$ and $\hbar \Omega = 15$ MeV is also shown (blue square). A linear extrapolation of the $\hbar \Omega = 13$ MeV and $\hbar \Omega = 17$ MeV results is used to determine an extrapolated alpha partial width of $C_l^{\text{SA-NCSM}} = 2.1(3) \times 10^8$ fm$^{-1/2}$. The error is given by the $\sim 13\%$ variation in $\hbar \Omega$. 
5.3.3 Reaction Rate and XRB Abundances

Using the narrow resonance approximation, given in Eq. (4.7)

\[ N_A\langle \sigma \nu \rangle_r = \frac{1.539 \times 10^{11}}{(\mu T_9)^{3/2}} e^{-11.605E_r/T_9} (\omega \gamma)_r, \]  

(5.19)

with the resonance strength given by

\[ (\omega \gamma)_r = \frac{2J_r + 1}{(2J_{A-\alpha} + 1)(2J_\alpha + 1)} \frac{\Gamma_\alpha \Gamma_\gamma}{\Gamma}, \]  

(5.20)

we compute the \( T_9 \)-dependent contribution to the \( \alpha + ^{16}\text{O} \) reaction rate through the 5.79 MeV \( 1^- \) resonance in \(^{20}\text{Ne} \). The reaction rate given in Eq. (5.19) takes as input the resonance strength \( (\omega \gamma)_r \) and resonance energy \( E_r \) in MeV. Note that the resonance strength \( (\omega \gamma)_r \) is dependent on the total angular momenta of the two clusters, \( J_\alpha, J_{A-\alpha} \), as well as the total angular momentum of the narrow resonance in the composite system through which the reaction occurs, \( J_r \). In addition, the resonance strength requires the alpha partial width \( \Gamma_\alpha \), which we compute, and the gamma decay branching ratio \( \Gamma_\gamma/\Gamma \). We use a branching ratio of \( 1.9 \times 10^{-4} \), which is estimated based on experimental data [197], but can be determined theoretically. Because the \( \Gamma_\alpha \sim \Gamma \), the resonance strength in Eq. (5.20) is actually driven by the much smaller value of \( \Gamma_\gamma \), which we do not calculate. However, since we take \( \Gamma_\gamma/\Gamma \) from experimental data, the reaction rate shown in Fig. 5.6 shows the difference in the rate as a result of the discrepancy in \( \Gamma_\alpha \).

5.3.4 Modules for Experiments in Stellar Astrophysics

The MESA code [2–6] is an open-source, modular code for one-dimensional stellar evolution with the capability to model various astrophysical environments, including simple stellar evolution of a main sequence star, as well as the complex mass accretion and explosive burning needed to describe XRBs. The modular nature of MESA allows for exceptionally versatile
Figure 5.6: A log-log plot of the reaction rate (cm$^3$/s/mol) determined with Eq. (5.19) as a function of the temperature (GK). The reaction rate determined with the extrapolated SA-NCSM/SU(3) alpha partial width $\Gamma_\alpha = 8(2)$ eV (red) is compared to the database reaction rate (blue). The uncertainty in the database rate is shown by the width of the blue curve.

uses of the code: users simply call in modules to drive various physical aspects of the system they intend to describe in their model.

The MESA release “Modules for Experiments in Stellar Astrophysics (MESA): Binaries, Pulsations, and Explosions” [4] included a model for a simple XRB with a constant accretion rate and consistent burning across the entire surface of the neutron star, based on GS 1826-24 [198], also known as the “clocked burster” [199]. This model is designed for a nuclear network of 305 isotopes, including proton rich isotopes up to $^{107}$Te, but is stable for a nuclear network consisting of 153 isotopes. For more details of the model and how it was fit to observed data, see section 5.2 of [4].

Using this reaction rate as input to MESA, we are able to determine the impact on the abundance pattern produced during a simulated XRB using reaction data determined from \textit{ab initio} wave functions. We use the 153-isotope nuclear network, which includes neutrons up to $^{56}$Fe$^3$. MESA includes all known reactions involving these nuclei, and rates are taken

\footnote{The network actually includes $^{138}$Ba as a flag for determining whether the simulation is unphysical, as XRB nucleosynthesis should not produce $^{138}$Ba.}
Figure 5.7: The difference between the initial mass fractions of the neutron star and the mass fractions 24 hours after the burst begins are shown for the MESA XRB simulation that uses the database rate (blue circles) and the MESA XRB simulation using the SA-NCSM calculated rate shown in Fig. 5.6 (red ×). The 24-hour period allows the system to burst a number of times, so that the sampled abundance pattern is the result of a series of bursts. All isotopes in the network with a mass fraction $> 10^{-10}$ are shown, and we label isotopes of interest. The inset shows a detailed look at the abundance pattern for isotopes of H, He, Mn, and Fe.
from the JINA REACLIB database [9]. We modify the rate for the $\alpha + ^{16}\text{O}$ reaction manually.

The difference between the initial mass fractions (i.e., masses given as a fraction of the total mass of the star) and the mass fractions a 24-hour period after the burst begins in simulation for the database reaction rate as compared to the theoretical rate we determine are shown in Fig. 5.7. In this time frame, the system undergoes a number of bursts, but is sampled in a quiescent phase after a burst. The overall abundance pattern is relatively unchanged, except for a slight decrease in burning of the $^1\text{H}$ and $^4\text{He}$ fuels, which translates directly to a decrease in production of iron and manganese isotopes, for the theoretical $\alpha + ^{16}\text{O}$ reaction rate. This does not appear to be related to an overall change in the production of $^{16}\text{O}$ or $^{20}\text{Ne}$, but does appear to change the abundances of some other $sd$-shell nuclei, particularly $^{30}\text{Si}$, $^{34}\text{S}$, and $^{38}\text{Ar}$, all of which have increased production with the change in the $\alpha + ^{16}\text{O}$ rate. The reduced theoretical alpha partial width, compared to the experimentally known width, results in a reduced $\alpha + ^{16}\text{O}$ reaction rate compared to the database rate. Because of this slight reduction in the reaction rate, alpha particles are apparently not burning as efficiently. As a result, some $sd$-shell nuclei are more abundant with the change in reaction rate, possibly because there are more alpha particles available for capture on isotopes other than $^{16}\text{O}$. Production of Fe and Mn, is reduced, but the overall pattern is only slightly affected by the deviations in the theoretical results.
6 Astrophysically Relevant Reactions

Using the framework laid out in Chapter 5, spectroscopic amplitudes and alpha widths are computed for a variety of nuclei of \( A = 6 - 19 \). Specifically, we consider the \( \alpha + d \rightarrow ^{6}\text{Li} \), \( \alpha + ^{8}\text{Be} \rightarrow ^{12}\text{C} \), \( \alpha + ^{9}\text{Be} \rightarrow ^{13}\text{C} \), \( \alpha + ^{12}\text{C} \rightarrow ^{16}\text{O} \), and finally the \( \alpha + ^{15}\text{O} \rightarrow ^{19}\text{Ne} \). Composite \( A \)-particle wave functions for each system are calculated in the NCSpM, using model spaces that are converged with respect to \( N_{\text{max}} \) (typically \( N_{\text{max}} = 20 \) is sufficient), and with the empirical estimate \( \hbar \Omega = 41/A^{1/3} \) MeV.

6.1 \( \alpha + d \rightarrow ^{6}\text{Li} \)

The \(^{2}\text{H}(\alpha, \gamma)^{6}\text{Li}\) radiative capture reaction is of interest both for answering questions about the production of \(^{6}\text{Li}\) in Big Bang nucleosynthesis (BBN), and because it involves two of the most fundamental building blocks in nuclear physics (deuterons and alpha particles).

The question of whether \(^{6}\text{Li}\) is produced in any significant abundance in BBN is somewhat open. In 2006, observations of \(^{6}\text{Li}\) absorption lines in quite old halo stars gave some evidence that the primordial abundance of \(^{6}\text{Li}\) was higher than previously thought [200]. A number of studies were conducted in response to this unexpected result, looking for possible explanations for an increase in \(^{6}\text{Li}\) production in the universe, including explanations involving physics beyond the standard model (for a review on beyond-standard-model physics solutions to the Lithium problems, see [201]). Other studies proposed that the original observation was artificially inflated due to convective Doppler shifts in stellar atmospheres causing line shifts that might be reasonably but incorrectly interpreted as being caused by the existence of \(^{6}\text{Li}\) [202, 203]. In 2014, the first direct measurement of \(^{2}\text{H}(\alpha, \gamma)^{6}\text{Li}\) at astrophysical energies was made at the LUNA 400 kV accelerator in Gran Sasso, Italy, and found a primordial \(^{6}\text{Li}/^{7}\text{Li}\) ratio of \( \sim 10^{-5} \), consistent with BBN predictions. Most existing evidence at this time indicates that \(^{6}\text{Li}\) is not produced in great quantities during the Big Bang, but the \(^{2}\text{H}(\alpha, \gamma)^{6}\text{Li}\) reaction remains of interest.

Both because of the efforts described above to understand the possible production of \(^{6}\text{Li}\) in BBN, and because the \( \alpha + d \) system is of fundamental interest to nuclear physics, this reaction
Figure 6.1: (a) The internal (solid line) and external (dashed line) wave function of the $\alpha + d$ wave function in the $gs$ of $^6$Li, and (b) spectroscopic amplitude for the 711-keV $3^+$ resonance for $\alpha + d \rightarrow ^6$Li. The exterior contribution (dashed) is dominated by the asymptotically oscillating Coulomb-Hankel function. The $^6$Li wave functions are calculated in the NCSpM with $N_{\text{max}} = 20$.

has been studied in a theoretical framework using cluster models with effective inter-cluster interactions [204], using the variational Monte Carlo method with realistic potentials [205], and in the $ab$ $initio$ NCSMC [146]. There are two main features of interest in this system that most studies consider: (1) the energy and width of the 711-keV $3^+$ resonance, and (2) the ratio of the $S$-wave ANC to the $D$-wave ANC (often denoted $\eta$) of the $\alpha + d$ configuration in the $^6$Li $gs$ wave function.

The spectroscopic amplitude for the 711-keV $3^+$ resonance is shown in Fig. 6.1(b). The associated partial width is $\Gamma_\alpha = 1.9$ keV (see Table 6.1), compared to the evaluated natural width $\Gamma = 24(2)$ keV. The NCSMC study does not report an alpha partial width, but determines the natural width of the $3^+$ state to be $\Gamma = 70$ keV [146]. A true comparison to the natural width directly requires a determination of the gamma decay width $\Gamma_\gamma$ through $E2$ values. This is in theory achievable within the reaction framework presented here, but is outside the scope of this work. It is promising, however, that the partial width is of the same order with the natural width, and doesn’t exceed the natural width.

We determine the ANC for the $^6$Li $gs$ using a NCSpM wave function, which has only $S$-wave contributions, so we cannot report on the ratio $\eta$ at present. A future study using SA-NCSM/Sp(3,\mathbb{R}) wave functions, which do have mixing of the $S$- and $D$-waves in the
ground state is in progress. Fig. 6.1(a) shows the $\alpha + d$ wavefunction in the $^{6}\text{Li}$ gs, with an ANC of 2.42 fm$^{-1/2}$ (see Table 6.2). This is slightly smaller than the experimentally measured $S$-wave contribution to the $^{6}\text{Li}$ gs at 2.91(9) fm$^{-1/2}$ [206], as well as the NCSMC $S$-wave ANC of 2.695 fm$^{-1/2}$ [146]. An evaluation of error introduced in the model will require more calculations, using the \textit{ab initio} SA-NCSM wave functions, and assessing the dependence of the result on the $\hbar\Omega$ and $N_{\text{max}}$ model parameters. As an initial evaluation, however, reproducing the order of magnitude of the ANC is very promising.

Table 6.1: Calculated maximum possible alpha partial width $\Gamma_\alpha$, compared to evaluated natural widths $\Gamma$. The wave functions were calculated in the NCSpM in a model space that shows convergece with respect to the $N_{\text{max}}$ parameter, and using the empirical estimate $\hbar\Omega = 41/A^{1/3}$ MeV.

<table>
<thead>
<tr>
<th>partitioning</th>
<th>max. $\Gamma_\alpha$</th>
<th>expt. $\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha + d \rightarrow ^{6}\text{Li} \quad 3^+ \quad (E_r = 711 \text{ keV})$</td>
<td>1.9 keV</td>
<td>24(2) keV [207]</td>
</tr>
<tr>
<td>$\alpha + ^{8}\text{Be} \rightarrow ^{12}\text{C} \quad 0^+ \quad (E_r = 287 \text{ keV})$</td>
<td>1.32 eV</td>
<td>9.3(9) eV [208]</td>
</tr>
<tr>
<td>$\alpha + ^{12}\text{C} \rightarrow ^{16}\text{O} \quad 4^+ \quad (E_r = 3.19 \text{ MeV})$</td>
<td>11.13 keV</td>
<td>26(3) keV [209]</td>
</tr>
<tr>
<td>$\alpha + ^{15}\text{O} \rightarrow ^{19}\text{Ne} \quad 3^+ \quad (E_r = 500 \text{ keV})$</td>
<td>$5.12 \times 10^{-6}$ eV</td>
<td>-</td>
</tr>
</tbody>
</table>

6.2 $\alpha + ^{8}\text{Be} \rightarrow ^{12}\text{C}$

Both $^{12}\text{C}$ and $^{16}\text{O}$ are alpha conjugate nuclei with strong 3- and 4-\alpha cluster substructures. As discussed in Chapters 2 and 3, understanding the alpha cluster substructure of $^{12}\text{C}$ – especially the Hoyle state – is one of the great open questions in nuclear cluster physics. The reaction rate for the triple alpha process itself still has not been measured directly, despite being one of the key energy-producing reactions in stars.

Here, we determine the spectroscopic amplitude and alpha partial width of the Hoyle state in $^{12}\text{C}$ within this framework, using a NCSpM wave function. The spectroscopic amplitude for this state has an extremely broad tail – the oscillatory behavior in the Coulomb-Hankel functions does not begin until $r > 40$ fm, as shown in the inset in Fig. 6.2. We determine an alpha partial width of 1.32 eV, which is a relatively small fraction of the total width of the state of 9.3(9) eV [210], but does reproduce the expected order of magnitude for the partial width. There is competition between the $\alpha + ^{8}\text{Be}$ decay mode and the breakup into
three alpha clusters. The extent to which the triple-alpha cluster configuration contributes is a matter of ongoing debate, although recent experimental results have indicated that the triple-alpha configuration contributes only as much as 0.043-0.047% to the decay of the Hoyle state [211,212]. A calculation of the natural width may require a coupled-channels approach that treats both the $\alpha + ^8\text{Be}$ channel and the $3\alpha$ channel, in addition to determining the gamma partial width $\Gamma_\gamma$.

Table 6.2: The maximum possible $C_2^2$ in fm$^{-1}$ calculated using Eq. (4.18). For $\alpha+d \rightarrow ^6\text{Li}$, experimental data is given for $C_1$ (fm$^{-1/2}$), so we compare directly with this. The bound state wave functions for the composite $A$-particle system are calculated in the NCSpM with model spaces that are converged with respect to the $N_{\text{max}}$ parameter, and using the empirical estimate $\hbar\Omega = 41/A^{1/3}$ MeV.

<table>
<thead>
<tr>
<th>partitioning</th>
<th>max. $C_2^2$ (fm$^{-1}$)</th>
<th>expt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha + ^9\text{Be} \rightarrow ^{13}\text{C}$ $1^-(gs)$</td>
<td>5.76 $\times 10^3$</td>
<td>-</td>
</tr>
<tr>
<td>$\alpha + ^{12}\text{C} \rightarrow ^{16}\text{O}$ $0^+(gs)$</td>
<td>6.73 $\times 10^4$</td>
<td>-</td>
</tr>
<tr>
<td>$\alpha + ^{12}\text{C} \rightarrow ^{16}\text{O}$ $0^+(6.05\text{MeV})$</td>
<td>3.11 $\times 10^6$</td>
<td>2.43 $\pm$ 0.30 $\times 10^6$ [196]</td>
</tr>
<tr>
<td>$\alpha + ^{12}\text{C} \rightarrow ^{16}\text{O}$ $2^+(6.92\text{MeV})$</td>
<td>1.81 $\times 10^{10}$</td>
<td>1.48 $\pm$ 0.16 $\times 10^{10}$ [196]</td>
</tr>
<tr>
<td>$\alpha + ^{12}\text{C} \rightarrow ^{16}\text{O}$ $1^-$(7.12MeV)</td>
<td>3.66 $\times 10^{28}$</td>
<td>4.39 $\pm$ 0.59 $\times 10^{28}$ [196]</td>
</tr>
<tr>
<td>$\alpha + ^{15}\text{O} \rightarrow ^{19}\text{Ne}$ $1^+(gs)$</td>
<td>4.57 $\times 10^6$</td>
<td>-</td>
</tr>
<tr>
<td>$\alpha + d \rightarrow ^6\text{Li}$ $1^+(gs)$</td>
<td>$C_1 = 2.42$ fm$^{-17/2}$</td>
<td>$C_1 = 2.91(9)$ fm$^{-17/2}$ [206]</td>
</tr>
</tbody>
</table>
Figure 6.3: (a) The internal (solid lines) and external (dashed lines) wave functions for $\alpha + ^{12}\text{C}$ in the ground state (red), the Hoyle-like $0^+$ state (grey), the first excited $1^-$ state (black), and the first excited $2^+$ state (blue) in $^{16}\text{O}$. All of these are bound with respect to the $^{12}\text{C} + \alpha$ threshold at 7.16 MeV; (b) The spectroscopic amplitude for the 10.36-MeV $4^+$ state in $^{16}\text{O}$ within the $\alpha + ^{12}\text{C}$ cluster framework. The exterior contribution (dashed) is dominated by the asymptotically oscillating Coulomb-Hankel function. Wave functions for the composite $^{16}\text{O}$ system are calculated with the NCSpM in an $N_{\text{max}} = 12$ model space.

6.3 $\alpha + ^{12}\text{C} \rightarrow ^{16}\text{O}$

The $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$ alpha capture reaction is of fundamental importance in nuclear astrophysics: once a significant amount of carbon is built up through the triple-$\alpha$ process in the helium burning phase of stellar evolution, the radiative capture of $\alpha$ particles on $^{12}\text{C}$ becomes statistically viable. This reaction essentially determines the relative abundance of $^{12}\text{C}$ and $^{16}\text{O}$ in the stellar core, which (1) constrains the $^{16}\text{O}(\alpha, \gamma)^{20}\text{Ne}$ reaction rate, (2) determines subsequent stellar burning phases, and (3) has impacts on the production of heavier isotopes in both quiescent and explosive burning processes. In addition, in XRB nucleosynthesis, the $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$ reaction rate has been identified as having a noticeable impact on simulated light curves, and a significant impact on ash composition [30].

This reaction rate is not known to the precision required for astrophysics simulations ($\sim 10\%$) [213], because direct measurements at astrophysically relevant energies have immeasurably low cross sections. The ANCs for a number of near-threshold bound states have been determined experimentally, including the 6.05-MeV $0^+$ state, the 6.92-MeV $2^+$ state, and the 7.12-MeV $1^-$, in an effort to indirectly determine the reaction rate [65, 196]. Here,
we calculate ANCs for the ground state and each of these excited states, as well as the alpha partial width through the 10.36 MeV $4^+$ state.

Wave functions for $\alpha + ^{12}\text{C}$ in bound states of $^{16}\text{O}$ are shown in Fig. 6.3(a). Note that for the ground state, the wave function has almost no tail – meaning there is very little information about the continuum in this state. The higher-lying $1^-$ state, the $2^+$ state, and the $0^+$ state just below the threshold are much more extensive, and are associated with much higher ANCs. It is states like these that may be used to determine alpha widths through indirect methods, as in Refs. [65,196]. The maximized ANCs for these states agree remarkably well – to within $2\sigma$ – with experimentally determined values for the 6.05 MeV $0^+$ state, the 6.92 MeV $2^+$ state, and the 7.12 MeV $1^-$ (see Table 6.2), despite the huge variation in the ANCs between states. Again, a $\pm1$ MeV shift in threshold energy introduces $< 10\%$ error to the calculation of the ANC.

The spectroscopic amplitude for the 10.36-MeV $4^+$ state in $^{16}\text{O}$ for $^{12}\text{C} + \alpha$ is shown in Fig. 6.3(b), and yields an alpha partial width of $\Gamma_{\alpha} = 11.13$ keV, which agrees with the order of magnitude of the experimental natural width of $\Gamma = 26(3)$ keV.

6.4 $\alpha + ^9\text{Be} \rightarrow ^{13}\text{C}$

In addition to alpha conjugate nuclei, the formalism is applied to the asymmetric cluster system $\alpha + ^9\text{Be} \rightarrow ^{13}\text{C}$. Specifically, $^{13}\text{C}$ can be modeled as a $3 - \alpha$ cluster system with an additional spare neutron helping to “glue” the alpha particles together in analogy to the $^9\text{Be}$ system, where the two alphas comprising an unstable $^8\text{Be}$ are “glued” together with a spare neutron [55].

Here, we compute the bound state wave function for the $\frac{1}{2}^-$ gs of $^{13}\text{C}$ and the associated ANC for $\alpha + ^9\text{Be}$. There are a number of states that are near the 10.6476-MeV $^9\text{Be} + \alpha$ threshold, which may contribute to the alpha-capture reaction rate, and a detailed analysis of all contributions would require a coupled-channels approach. The ground state of $^{13}\text{C}$ has essentially no contribution from the continuum, as it is very bound with respect to the alpha capture threshold. The ANC is $C_I^2 = 5.76 \times 10^3 \text{ fm}^{-1}$ for the $^{13}\text{C}$ gs (see Table 6.2).
Figure 6.4: The internal (solid line) and external (dashed line) wave function of the $\alpha + {}^9\text{Be}$ system in the ground state of $^{13}\text{C}$. The $^{13}\text{C}$ gs wave function is calculated with the NCSpM in an $N_{\text{max}} = 16$ model space.

6.5 $\alpha + {}^{15}\text{O} \rightarrow {}^{19}\text{Ne}$

We also consider the CNO breakout reaction $^{15}\text{O}(\alpha,\gamma)^{19}\text{Ne}$ through the 4.03 MeV $3/2^+$ state in $^{19}\text{Ne}$, which has an asymmetric cluster structure. As discussed in Chapter 2, this is one of the most important reactions for modeling XRB nucleosynthesis: it has been identified as one of the reaction rates to which XRB lightcurves and abundance patterns are most sensitive in multiple studies [29, 30], and has been seen to impact burst recurrence in models of XRBs [31].

The $^{15}\text{O}(\alpha,\gamma)^{19}\text{Ne}$ reaction is expected to predominantly go through the 500-keV $3/2^+$ resonance in $^{19}\text{Ne}$, although there are other nearby resonances that are not well studied – possible $7/2^-$ and $9/2^-$ states at 4.1 MeV and 4.2 MeV, whose order is not yet experimentally verified. An $ab\ initio$ SA-NCSM study of the structure of $^{19}\text{Ne}$ has recently provided preliminary results, placing the $9/2^-$ state below the $7/2^-$ [214]. Here, we calculate the spectroscopic amplitude and alpha partial width for only the $3/2^+$ state mentioned above. A future study may make use of the SA-NCSM/SU(3) wave functions presented in Ref. [214] to determine the partial widths of these resonances as well.

The partial width of the $3/2^+$ state in $^{19}\text{Ne}$ using a NCSpM wave function with $N_{\text{max}} = 10$ and $\hbar \Omega = 41/A^{1/3} \approx 15$ MeV is very small: $\Gamma_\alpha = 5.12 \times 10^{-6} \text{ eV}$. The spectroscopic amplitude
Figure 6.5: (a) The internal (solid line) and external (dashed line) wave function for $^{15}\text{O} + \alpha$ in the ground state of $^{19}\text{Ne}$. (b) The spectroscopic amplitude for the 500 keV $3/2^+$ resonance for $\alpha + ^{15}\text{O} \rightarrow ^{19}\text{Ne}$. The exterior contribution (dashed) is dominated by the asymptotically oscillating Coulomb-Hankel function, shown in the inset. $^{19}\text{Ne}$ wave functions are calculated with the NCSpM in an $N_{\text{max}} = 16$ model space.

associated with this state is shown in Fig. 6.5(b). The $\alpha + ^{15}\text{O}$ reaction has been studied in the lab, with experiments in inverse kinematics putting upper bounds on the $\Gamma_\alpha/\Gamma_\gamma$ branching ratio [215] and the $\Gamma_\alpha/\Gamma$ branching ratio [216] for low-lying states. In particular, the $3/2^+$ branching ratio has been bounded to $\Gamma_\alpha/\Gamma < 10^{-4}$. There is still a good deal of uncertainty regarding the partial width of this state, and ongoing experimental efforts intend to address this uncertainty. There are a number of experimentally-determined upper bounds for the alpha branching ratio, but there is only one experimental measurement of the branching ratio, $\Gamma_\alpha/\Gamma = 2.9 \pm 2.1 \times 10^{-4}$ [217]. Although the 2011 sensitivity study found Type I XRBs to be insensitive to the $^{15}\text{O}(\alpha,\gamma)^{19}\text{Ne}$ reaction rate (in contrast to [30]), Davids et al. did call into question the quality of the measurement by Tan et al. [218]. There is no experimental data for the ANC for the $gs$ of $^{19}\text{Ne}$. We determine the $gs$ ANC to be $C_1^2 = 4.57 \times 10^6 \text{ fm}^{-1}$ (see Table 6.2). The associated bound state wave function is shown in Fig. 6.5(a).

Using the alpha width $\Gamma_\alpha = 5.12 \times 10^{-6} \text{ eV}$, and assuming the $\Gamma_\gamma/\Gamma \approx 1$ (true for $\Gamma_\gamma >> \Gamma_\alpha$), we calculate a reaction rate for $\alpha + ^{15}\text{O} \rightarrow ^{19}\text{Ne}$ with the narrow resonance approximation of Eq. (4.7). The REACLIB database rate for this reaction is an evaluated rate, and our calculated rate is 5 orders of magnitude smaller than the database rate. The
Figure 6.6: The difference between the initial mass fractions of the neutron star and the mass fractions 12 hours after the burst begins are shown for the MESA XRB simulation that uses the database rate (blue circles) and the MESA XRB simulation using the NCSpM calculated rate (red ×). Within the 12-hour period, two bursts occur. All isotopes in the network with a mass fraction $> 10^{-10}$ are shown, and we label isotopes of interest. The inset shows a detailed look at the abundance pattern for isotopes of H, He, Mn, and Fe.

reaction rate is used in the same MESA simulation of an XRB discussed in Chapter 5 to determine impact on XRB abundances, shown in Fig. 6.6.

Although we see some more significant changes in abundances, here, the overall difference is surprisingly still quite small. The most notable changes are a fairly significant decrease in hydrogen burning as a result of the new reaction rate, and a significant decrease in the production of the isotopes $^{22}$Na and $^{54}$Fe. The discrepancy in abundances of the $^{30}$Si and $^{34}$S is reversed from the $\alpha + ^{16}$O case – the production of both isotopes is slightly suppressed. It is interesting to note that, although a previous sensitivity study by Cyburt et al. indicated that the production of $^{12}$C may be noticeably impacted by the $^{15}$O($\alpha, \gamma$)$^{19}$Ne rate [30], we find no impact on the abundance of $^{12}$C, here.

Impacts on abundances determined in Ref. [30] are determined within the Kepler burst model, which is designed for the closed-source Kepler code [7]. The results we show here
are determined with the an XRB simulation described in section 5.3.4 built for use with MESA. The initial conditions for the Kepler burst model and the MESA XRB simulation may be very different, so a direct comparison of results is difficult. In any case, the current expectation is that the \(^{15}\text{O}(\alpha, \gamma)^{19}\text{Ne}\) breakout reaction should have a significant impact on XRB abundances, lightcurves, and burst recurrence, so this discrepancy bears further investigation.

In short, we present alpha widths and ANCs for a number of cluster systems with \(A = 6 - 19\). Calculated alpha partial widths reproduce the order of magnitude for experimentally known total widths in all cases where experimental data is known. We find remarkable agreement for the ANCs, in particular, the calculated \(\alpha + ^{12}\text{C} \rightarrow ^{16}\text{O}\) ANCs agree to within \(2\sigma\) with measured ANCs for the 6.05-MeV Hoyle-like \(0^+\), the 6.92-MeV \(2^+\) state, and the 7.12-MeV \(1^-\) state. We predict, for the first time within a no-core shell model framework, the alpha partial widths for the \(^{12}\text{C}\) Hoyle state, and the 500-keV \(3/2^+\) resonance in \(^{19}\text{Ne}\), both of which are of particular interest to nuclear astrophysics for their impact on nucleosynthesis.
7 Conclusion

This work outlines a new many-body reaction theory with the ability to determine asymptotic normalization coefficients (ANCs) and partial widths using \textit{ab initio} wave functions. Alpha partial widths are used to determine \(\alpha\)-capture reaction rates for narrow resonances in astrophysically important systems.

We validate the theory for the highly-clustered \(^{20}\text{Ne}\) system, including the ANC for the \(^{20}\text{Ne}\) ground state, the width of the 1.06 MeV \(1^-\) resonance in \(^{16}\text{O} + \alpha \rightarrow ^{20}\text{Ne}\), and the \(^{16}\text{O}(\alpha, \gamma)^{20}\text{Ne}\) reaction rate through this state. Because the \(^{16}\text{O}(\alpha, \gamma)^{20}\text{Ne}\) reaction rate is dominated by the contribution through this resonance at temperatures relevant to XRBs, we use a reaction rate determined from \textit{ab initio} wave functions in a MESA simulation of an XRB to determine the impact on the abundance pattern. Finally, our results for a number of systems of mass \(A = 6 - 19\) show the broader applicability of this theoretical framework to determine reaction data, including alpha partial widths and ANCs, for various systems that have a significant impact on astrophysical models. Our calculations are consistent with experimental results for alpha-conjugate nuclei, asymmetric cluster systems, and even-odd nuclei, indicating that the model is not restricted to only simple alpha-conjugate systems. We report exciting first results within a no-core shell model framework for the alpha partial width of the important \(3/2^+\) state in \(^{19}\text{Ne}\), which may significantly impact models of XRB nucleosynthesis.

Although the work presented here centers on \(\alpha\)-capture reactions because of their importance to astrophysics, the theory is not limited to reactions involving alpha clusters: the current status of the theoretical framework is fully applicable to single-particle clusters (e.g., for studies of radiative proton capture), deuterons, and heavier clusters (e.g., one could study the \(^{12}\text{C} + ^{12}\text{C}\) system). Future work will aim to expand the theoretical framework in a number of ways, including introducing excitations in the individual clusters of the system, and introducing more richness to the description of the composite system through the inclusion of more symplectic irreps.
Appendix A: Derivation of a Recursive Overlap Formula

The spectroscopic amplitude in Eq. (5.13) is dependent on the overlap

\[ \mathcal{O} = \langle (A)\tilde{\alpha}\sigma_0\tilde{n}_0\rho_0\omega_0\Omega_0 | (\alpha\omega; n(n 0))\rho_0\omega_0\Omega_0 \rangle \]  

(7.1)

between a symplectic wave function for the composite $A$-particle system and a cluster basis wave function for the two-cluster system comprised of an $a$-particle cluster and an $(A - a)$-particle cluster. Our aim is to determine a recursive expression for the overlap, so that, e.g., the term with $n$ excitations in the relative motion is determined directly from the overlap for $n - 2$ excitations. The symplectic lowering operator lowers a symplectic state by two excitations. Here, we will determine the action of the symplectic lowering operator on a cluster basis state.

Consider the symplectic lowering operator $\mathcal{B}^{(02)}_{\Omega_B}(\bar{\zeta})$ acting on the cluster state:

\[ \mathcal{B}^{(02)}_{\Omega_B} |(\alpha\omega; n(n 0))\rho_0\omega_0\Omega_0 \rangle \]

\[ = \sum_{\omega', \omega, \rho_0' \rho_0 \omega_0' \omega_0} |(\omega'; \omega')\rho_0'\omega_0'\Omega_0'\rangle \langle (\omega'; \omega')\rho_0'\omega_0'\Omega_0' | \mathcal{B}^{(02)}_{\Omega_B} |(\alpha\omega; n(n 0))\rho_0\omega_0\Omega_0 \rangle, \]  

(7.2)

where we have introduced the completeness relation for the cluster basis on the right hand side. Considering the overlap between the state $\mathcal{B}^{(02)}_{\Omega_B} |(\alpha\omega; n(n 0))\rho_0\omega_0\Omega_0 \rangle$ and a generic symplectic basis state $|(A)\tilde{\alpha}\sigma_0\tilde{n}_0\rho_0\omega_0\Omega_0 \rangle$, and inserting the symplectic basis completion,

\[ \sum_{n_0' \rho_0' \omega_0' \Omega_0'} \langle (A)\tilde{\alpha}\sigma_0\tilde{n}_0\rho_0\omega_0\Omega_0 | \mathcal{B}^{(02)}_{\Omega_B} |(\alpha\omega; n(n 0))\rho_0\omega_0\Omega_0 \rangle \]

\[ = \sum_{\omega', \omega, \rho_0' \rho_0 \omega_0' \Omega_0} \langle (A)\tilde{\alpha}\sigma_0\tilde{n}_0\rho_0\omega_0\Omega_0 |(\omega'; \omega')\rho_0'\omega_0'\Omega_0' \rangle \]

\[ \times \langle (\omega'; \omega')\rho_0'\omega_0'\Omega_0' | \mathcal{B}^{(02)}_{\Omega_B} |(\alpha\omega; n(n 0))\rho_0\omega_0\Omega_0 \rangle, \]  

(7.3)

we have an expression that relates the expectation value of the symplectic lowering operator
in the symplectic basis to the expectation value of the symplectic lowering operator in the cluster basis. For orthonormal states with good quantum numbers $\rho_\omega \Omega$, the overlaps

$$\langle \bar{\alpha}_\sigma \bar{n}_0 \bar{\rho}_0 \bar{\omega}_0 \bar{\Omega}_0 | \langle (\omega'; \omega'_n) \rho'_0 \omega'_0 \Omega'_0 \rangle and \langle \bar{\alpha}_\sigma \bar{n}_0 \bar{\rho}_0 \bar{\omega}_0 \bar{\Omega}_0 | (\omega; n(0)) \rho_0 \omega_0 \Omega_0 \rangle$$

are only nonzero for the cases when $\bar{\rho}_0 = \rho'_0$, $\bar{\omega}_0 = \omega'_0$, $\bar{\Omega}_0 = \Omega'_0$, $\rho''_0 = \rho_0$, $\omega''_0 = \omega_0$, and $\Omega''_0 = \Omega_0$.

In order to determine the action of the symplectic lowering operator on a cluster basis state, we must first consider the coordinates in which the lowering operator is written. In the relative coordinates used by the NCSpM, the lowering operator can be separated into two pieces: a lowering operator that acts only on the cluster coordinates $B_{\Omega_B, c}^{(02)} = B_{\Omega_B}^{(02)} (\vec{\zeta}_1, \ldots, \vec{\zeta}_{A-1})$ and a lowering operator that acts only on the relative motion coordinate $B_{\Omega_B, \text{rel}}^{(02)} = B_{\Omega_B}^{(02)} (\vec{r}_{A-a})$ (see Appendix B). Using this, we can rewrite the matrix element of the lowering operator in the cluster basis into two terms

$$\langle (\omega'; \omega'_n) \rho'_0 \omega'_0 \Omega'_0 | B_{\Omega_B, c}^{(02)} | (\omega; n(0)) \rho_0 \omega_0 \Omega_0 \rangle = \sum_{\Omega''_n, \Omega_n} \langle \omega' \Omega'_n; \omega'_n \Omega'_n | \omega'_0 \Omega'_0 \rangle \rho'_0 \langle \omega \Omega; (n(0)) \Omega_n | \omega_0 \Omega_0 \rangle \rho_0$$

$$\times [\langle \omega' \Omega' | B_{\Omega_B, \text{rel}}^{(02)} | \omega \Omega \rangle \delta_{\omega'_n(n(0))} \delta_{\Omega'_n \Omega_n} + \langle \omega' \Omega'_n | B_{\Omega_B, \text{rel}}^{(02)} | n(0) \Omega_n \rangle \delta_{\omega' \Omega' \Omega} ], \quad (7.4)$$

where we have also decoupled from $\omega'_0$ and $\omega_0$, and dropped the notation $\alpha$ for simplicity.

For clusters described by the bandhead of a symplectic irrep, $B_{\Omega_B}^{(02)} | \omega \Omega \rangle = 0$, and so only the second term is nonzero. The remaining term represents the action of the symplectic lowering operator on the relative motion between the two clusters, alone. After reducing the matrix element on the left hand side using the SU(3) Wigner-Eckart Theorem (see, e.g., Eq. (C27) in [219]), and collecting reduced Wigner coefficients into an SU(3) Racah coefficient
using equation (C20) from [219], Eq. (7.4) is expressed simply as

\[ \langle (\omega'; \omega_n') \rho_0 \omega_0 \| B^{(02)} \| (\omega; n(0)) \rho_0 \omega_0 \rangle_{\rho_B} = \sum_{\rho_B} U[\omega(n(0)\omega'_0(02); \omega_0 \rho_0 \rho'_B; \omega'_n \rho_B \rho_0'] \langle \omega'_n \| B^{(02)}_{rel} \| n(n(0)) \rangle_{\rho_B} \delta_{\omega_0} \]  

(7.5)

From Eq. (12) in [190], there is only one nonzero matrix element of \( \langle \omega'_n \| B^{(02)}_{rel} \| n(n(0)) \rangle_{\rho_B} \); namely, the matrix element \( \langle n - 2(n - 20) \| B^{(02)}_{rel} \| n(0) \rangle_{\rho_B} \). This reduced matrix element is known analytically. Specifically, using Eq. (28) of Ref. [220],

\[ \langle N_0 + n + 2 (\lambda_0 + n + 2 \mu_0) \| A^{(20)} \| N_0 + n (\lambda_0 + n \mu_0) \rangle = \left( \frac{1}{3} (N_0 + 2 \lambda_0 + \mu_0 + \frac{3}{2} n)(2 + n) \right)^{1/2}, \]  

(7.6)

and with

\[ \langle N'(\lambda' \mu') \| B^{(02)} \| N(\lambda \mu) \rangle = (-)^{\lambda' + \mu'} (\dim(\lambda \mu))^{1/2} \langle N(\lambda \mu) \| A^{(02)} \| N'(\lambda' \mu') \rangle^*, \]  

(7.7)

then for the \( \langle n - 2(n - 20) \| B^{(02)}_{rel} \| n(0) \rangle_{\rho_B} \) matrix element, we have

\[ \langle n - 2(n - 20) \| B^{(02)}_{rel} \| n(0) \rangle_{\rho_B} = \sqrt{\dim(n 0)}. \]  

(7.8)

This agrees with the value used in Eq. (24c) of Ref. [94].

Returning to Eq. (7.3), the matrix element of the symplectic lowering operator between the symplectic states on the left hand side can be expressed as [221]:

80
\begin{equation}
\langle (A)\tilde{\alpha}\sigma_0\tilde{n}_0\tilde{\rho}_0\tilde{\omega}_0\tilde{\Omega}_0|B^{(02)}_{\Omega_0}|\tilde{\alpha}\sigma_0\tilde{n}_0''\rho_0\omega_0\Omega_0 \rangle
= \sum_{\rho} \langle \omega_0\Omega_0; (0 2)\Omega_B|\tilde{\omega}_0\tilde{\Omega}_0 \rangle \rho [\Delta \Omega_K(n_0\omega_0, \tilde{n}_0\tilde{\omega}_0)]^{1/2}
\times (-)^{\tilde{\omega}_0-\omega_0} U[\sigma_0n_0\tilde{\omega}_0(0 2); \omega_0\rho_0 1\tilde{n}_0 1\tilde{\rho}_0](\tilde{n}_0||B^{(02)}||n_0),
\end{equation}

where the final fully reduced matrix element $(\tilde{n}_0||B^{(02)}||n_0)$ is computed using the expressions in Table I of Ref. [222].

Substituting Eqs. (7.9) and (7.5) back into Eq. (7.3), we determine the recursion relation in Eq. (5.16) for determining the overlap between cluster and symplectic basis states.

The base case for the recursion is given for the $N_{n_0} = 0$ case:

\begin{equation}
\langle (A)\tilde{\alpha}\sigma_00(0 0)1\sigma_0\Omega_0|\omega; n_{\text{min}}(n_{\text{min}} 0)1\sigma_0\Omega_0 \rangle = 1,
\end{equation}

where $n_{\text{min}} = N_{\sigma} - N_{\omega}' - N_{\omega}'' - 1.5$. 
Appendix B: Separation of the Symplectic Lowering Operator

We intend to show that $B^{(0)}_{LM}$ can be written as a sum of two terms,

$$B^{(0)}_{LM}(\vec{\zeta}) = B^{(0)}_{LM}(\vec{\zeta}_1, \ldots, \vec{\zeta}_{A-1}) + B^{(0)}_{LM}(\vec{r}_{A-a,a})$$  \hspace{1cm} (7.11)

one that acts on the two clusters, and a second term that acts only on the relative motion between the two. The symplectic lowering operator is the conjugate to the symplectic raising operator: $B^{(0)}_{LM} = (-)^{L-M}(A_{L,M}^{(0)})^\dagger$. It suffices to show this separation for the symplectic raising operator.

The symplectic raising operator can be written in terms of the dimensionless HO raising and lowering operators, $b_{j\alpha}^{(1)} = \frac{1}{\sqrt{2}}(r_{j\alpha} - ip_{j\alpha})$ and $b^{(0)}_{j\alpha}$ respectively, for each particle $j$ in an $A$-particle system. The position and momentum coordinates of the $j^{th}$ particle in the lab frame are $\vec{r}_j$ and $\vec{p}_j$, respectively, and $\alpha = 1, 2, 3$ enumerates the three spatial directions. The raising operator is written for the relative coordinates $\vec{\zeta}$:

$$A^{(2)}_{LM}(\vec{\zeta}) = \frac{1}{\sqrt{2}} \sum_{i=1}^{A} \{b_{i\alpha}^{\dagger} \times b_i^{(2)}\}_{LM} - \frac{1}{\sqrt{2}A} \sum_{s,t=1}^{A} \{b_{s\alpha}^{\dagger} \times b_t^{(2)}\}_{LM}$$

$$= A^{(2)}_{LM}(\vec{r}) \pm A^{(2)}_{LM}(\vec{R}).$$  \hspace{1cm} (7.12)

The sums over $i, s, t$ are sums over the $A$ particles in the system, $\vec{r} = \{\vec{r}_1, \ldots, \vec{r}_A\}$ are the laboratory coordinates for the particles, and $\vec{R}$ is the center of mass of the $A$-particle system (see Fig. 5.1). The notations $A^{(2)}_{L,M}(\vec{r})$ and $A^{(2)}_{L,M}(\vec{R})$ are introduced to denote the raising operator for the $A$-particle system in the laboratory frame, and the CM contribution to the raising operator, respectively. Note, that Eq. (7.12) implies

$$A^{(2)}_{L,M}(\vec{r}) = A^{(2)}_{L,M}(\vec{\zeta}) + A^{(2)}_{L,M}(\vec{R}).$$  \hspace{1cm} (7.13)

Then, the sum over the $A$ particles in the laboratory frame can be separated into two
sums over the particles in each of the two clusters,

\[
A^{(20)}_{LM}(\vec{r}) = \frac{1}{\sqrt{2}} \sum_{i=1}^{A} \{ b_i^\dagger \times b_i^\dagger \}_{LM}^{(20)} + \sum_{i=A-a+1}^{A} \{ b_i^\dagger \times b_i^\dagger \}_{LM}^{(20)}
\]

\[
= A^{(20)}_{LM}(\vec{r}) + A^{(20)}_{LM}(\vec{r}'')
\]

(7.14)

where each of the sums is rewritten as a raising operator for a single cluster in the laboratory frame. The coordinates \(\vec{r}' = \{ \vec{r}_1, \ldots, \vec{r}_{A-a} \}\) and \(\vec{r}'' = \{ \vec{r}_{A-a+1}, \ldots, \vec{r}_A \}\) are the laboratory frame coordinates for the particles in each of the two clusters.

Each of these laboratory frame cluster raising operators can be written as a sum of a relative contribution and a CM contribution, as in Eq. (7.13), so that the total laboratory frame raising operator is

\[
A^{(20)}_{LM}(\vec{r}) = A^{(20)}_{LM}(\vec{\zeta}') + A^{(20)}_{LM}(\vec{R}') + A^{(20)}_{LM}(\vec{\zeta}'') + A^{(20)}_{LM}(\vec{R}'')
\]

(7.15)

and the raising operator in relative coordinates for the total system is

\[
A^{(20)}_{LM}(\vec{\zeta}) = A^{(20)}_{LM}(\vec{\zeta}') + A^{(20)}_{LM}(\vec{R}') + A^{(20)}_{LM}(\vec{\zeta}'') + A^{(20)}_{LM}(\vec{R}'') - A^{(20)}_{LM}(\vec{R}).
\]

(7.16)

Note that the \(A^{(20)}_{LM}(\vec{\zeta}')\) and \(A^{(20)}_{LM}(\vec{\zeta}'')\) are exactly the terms we want – each of them would act independently on a single cluster, and so

\[
A^{(20)}_{LM}(\vec{\zeta}_1, \ldots, \vec{\zeta}_{A-1}) = A^{(20)}_{LM}(\vec{\zeta}') + A^{(20)}_{LM}(\vec{\zeta}'').
\]

(7.17)

We need to show that the second line of Eq. (7.16) simplifies to a term that acts only on the relative motion between the two clusters.

Consider the laboratory frame system of two particles, with laboratory frame coordinates
\( \vec{R}' \) and \( \vec{R}'' \). Then, using Eq. (7.13),

\[
A^{(20)}_{LM}(\vec{R}') + A^{(20)}_{LM}(\vec{R}'') = A^{(20)}_{LM}(\vec{r}_{A-a,a}) + A^{(20)\text{CM}}_{LM}(\vec{R}). \tag{7.18}
\]

Then, the raising operator in relative coordinates for the total system is

\[
A^{(20)}_{LM}(\vec{\zeta}) = A^{(20)}_{LM}(\vec{\zeta}_1, \ldots, \vec{\zeta}_{A-a-1}) + A^{(20)}_{LM}(\vec{r}_{A-a,a}) \tag{7.19}
\]

where the CM terms cancel, and the result is what we desired to achieve in Eq. (7.11).
References


[143] Jérémie Dohet-Eraly, Petr Navrátil, Sofia Quaglioni, Wataru Horiuchi, Guillaume Hupin, and Francesco Raimondi. $^3\text{He}(\alpha,\gamma)^7\text{Be}$ and $^3\text{H}(\alpha,\gamma)^7\text{Li}$ astrophysical $S$ factors from the no-core shell model with continuum. *Physics Letters B*, 757:430–436, 2016.


Vita

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