Coupled-cluster theory for open shell nuclei

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Chapter 1

Introduction

We wish to understand the structure of matter. This is an enterprise that has occupied natural philosophers for millennia. In pre-Socratic Greece, Thales of Miletus envisioned water as the foundation of all matter, while contemporaries both in Greece and India formed the idea of an atom as the smallest undividable unit of matter. And although the view of what constitutes the smallest units of matter has changed since, the idea that all matter can be reduced to its fundamental constituents is one of the pillars of modern particle physics.

While the attempt to describe matter using the fundamental degrees of freedom may sound appealing, in practical calculations such an approach is not possible. A successful description of matter can only be accomplished by using the tools and degrees of freedom that are relevant for the properties under investigation. This changes as the energy in the observation process changes. Thus, the study of matter can be divided into many different disciplines, ranging from the microscopic at high energies to the macroscopic at low energies.

In this thesis, the focus is on the theoretical description of the structure of atomic nuclei, so-called low energy nuclear physics. At this scale, the nucleus is considered a self-bound system of protons and neutrons, collectively called nucleons. This system is classified as a non-relativistic quantum many-body system and is studied by quantum many-body methods that solve the many-body Schrödinger equation to obtain the binding energy, related to the mass

of the nucleus and the low-energy excitation spectrum. If the wave function is obtained, other properties like spatial extension, charge distribution, transition probabilities etc. can also be calculated. All these properties are low energy properties compared to the mass of the nucleus and are related to the internal organization of the nucleons.

This thesis is divided into two parts. In section 2, the focus in on developing a method used to solve the problem and its convergence properties. It is applicable to nuclei that can be described as two particle attached to or removed from a closed (sub-)shell nucleus. Two articles are presented where the method is evaluated. The first is a proof-of-principle, where the formal theory is presented and a calculation is performed in a very small model space. The second paper presents a set of analytical optimizations that exploit the rotational symmetry of the Hamiltonian. This allows calculations to be performed in very large model spaces where converged results are obtained. Thus, the only error introduced is due to the approximations done in the method itself.

In section 3, the focus is on the application of the method. As it is a part of a larger class of methods, where each solve the problem for a specific subset of nuclei, multiple methods were used to examine the properties of the isotopic chains of oxygen and calcium. These studies are presented in two separate papers.

Finally, section 4 contains some final remarks and a brief discussion of the road ahead. All four papers that are a part of this thesis, are included in the appendix.

Chapter 2

Modelling the nucleus

2.1 Relevant degrees of freedom

The reductionist approach to low-energy nuclear structure, would be to model the nucleus using whatever is currently considered the fundamental degrees of freedom. Today, that would be quarks and gluons, interacting through the strong, weak and electromagnetic force, as well as gravity. The focus of this thesis is on practical calculations and such an approach is not practically possible. There are several reasons for this. First, limits imposed on numerical precision would deny the simultaneous treatment of all forces. The effects of gravity and the weak interaction would be completely invisible compared to the effects of the remaining two forces. Second, the calculations that would have to be performed, are so complex that limitations in our current level of technology will not allow them. If this was not an issue, limits on the number of floating point operations that can be performed per second (FLOPS), would result in calculations that would basically never finish. Moreover, the precision required of experimental data to evaluate such a calculation, would have to be orders of magnitude better than what is possible today. Instead, we try to find the relevant degrees of freedom for any given property or process. If a solvable model can be worked out, it may provide not only valuable insight, but also clues to create a more accurate model for the next generation of tools.

The relevant degrees of freedom in low-energy nuclear physics are protons

and neutrons, collectively called nucleons. They are part of a larger family of particles called baryons, but only the nucleons are stable enough to survive and form the bound structures we call nuclei. In this model, the interaction between nucleons is mediated by a class of particles called mesons. The range of the interaction is determined by the mass of the meson involved, where the lightest mesons, called the pions, are considered dominant at long range or low energies. Both the baryons and the mesons are part of an even bigger family of particles called hadrons. All hadrons are composite particles, where the constituents are quarks and gluons. It is the interaction between the quarks and gluons, that is ultimately responsible for nuclear binding.

In the standard model of particle physics, quantum chromo dynamics (QCD) is the field theory that describes the strong interaction between quarks and gluons. The quarks come in six different flavours, but only the two lightest quarks, named up and down, make up the nucleons. In the larger picture, the up and down quarks are part of the first generation of particles together with the electron and the electron-neutrino, that are the constituents of all ordinary matter. The gluons are considered the force carriers mediating the strong nuclear force.

The quarks and gluons carry a strong charge, called color. This charge comes in three different values along with their anti-particle complements. Each quark carries only a single color. The color content of gluons is more complicated. Here, the color charge is a linear combination of different colors and anti-colors. There are only eight orthogonal combination, making up the color octet of gluons.

There are two properties of QCD that are important when a model of the nucleus is attempted. One requires, while the other justifies the use of hadrons as the relevant degrees of freedom at low energies. The property of asymptotic freedom is a feature of QCD and it means that the coupling strength between quarks and gluons becomes weaker at higher energies. This enables a solution using perturbation theory, analogous to quantum electro dynamics (QED). At low energies, the interaction is very strong, with the consequence that low-energy QCD is non-perturbative. This means that a perturbative expansion in terms of the interaction, does not converge. The strong force is the only force that does not decrease in strength at long range and an exact solution of the field equations is necessary. Such a solution is certainly possible. In lattice QCD (LQCD), space-time is modelled as a

four-dimensional hypercube, where the field equations are solved using the path integral formalism. Using Monte Carlo integration, the integral kernel is only evaluated at certain points on the hypercube, called the grid points. A fixed distance between the grid points, called the lattice spacing, impose a minimum spacing between particles. This is effectively a momentum cutoff, since the lattice spacing has to be small enough to resolve the structure of the wave function. In addition, the total number of points on the hypercube is limited by available hardware, which sets an upper limit to the size of the hypercube. An additional restriction is set by the mass of the particles to be included, as the hypercube must be able to contain them. The Compton wavelength of a point particle is inversely proportional to its mass, so the size of the hypercube sets a lower limit on the mass of the particles. Efforts have been made to calculate properties of the nuclear interaction directly using LQCD [1–3], but it is still necessary to use large quark masses, resulting in a pion mass of about 350MeV. This is too large for a reliable extrapolation to experimental masses. Thus, the explicit treatment of quark degrees of freedom in a nucleus is not possible at present and requires a model where the nucleons are considered the relevant degrees of freedom.

Due to the strong interaction strength at long range, QCD displays a property called confinement. Free quarks are never observed, but are confined to form hadrons. It is important to realize that the hadrons carry no color charge. Quarks and anti-quarks combine in such a way, as to make color neutral composite particles. A quark and an anti-quark of the same color combine to form mesons, while three quarks with different colors combine to form baryons. Thus, the complex interaction observed between nucleons and mesons is only a residual interaction between quarks and gluons. This is completely analogous to the residual electromagnetic interaction observed between neutral atoms and molecules. Only at very high energies is the structure of hadrons visible to a probe, which justifies the use of hadrons as the relevant degrees of freedom in low-energy nuclear physics.

2.2 The nuclear interaction

The nuclear interaction is not known to us. There is no analogue to the Coulomb potential between electromagnetically charged particles, that acts

between nucleons. This is because the nucleons are effective degrees of freedom, with complex interactions that must be fitted to experimental data to produce reliable results. We have many models with varying numbers of parameters, that reproduce nucleon-nucleon observables to a very high precision. Models based on meson exchange (see Machleidt [4] for an excellent introduction) are giving way to modern potentials based on the approximate chiral symmetries of QCD [5, 6]. While all models reproduce two-nucleon observables, for systems with more than two nucleons, the relevant observables are not reproduced. The nucleon-nucleon (NN) force is considered insufficient to reproduce relevant observables.

Many take this as a clue that nucleons are not the only relevant degrees of freedom in the nucleus. Maybe pions and nucleon resonances have to be treated explicitly in any calculation involving more than two nucleons. The current approach is to model the missing physics by introducing three-nucleon forces (3NF). If this proves insufficient, maybe four-nucleon forces needs to be included as well. However, modern *ab initio* methods (see Leidemann and Orlandini [7] for a recent review) are barely capable of exploring the effects of three-nucleon forces in the lightest nuclei. It will take some time before a level of precision is reached where eventual four-nucleon forces are deemed necessary. The experimentally observed hierarchy of many-body forces ensures that we handle three-nucleon forces correctly, before contemplating forces with higher particle rank.

In the past fifteen years, a direct connection between the nuclear interaction and QCD has been established. Using the framework of effective field theory (EFT), chiral perturbation theory has unveiled a consistent picture of nuclear forces. Here, many-body forces emerge naturally and are all treated equally. The perturbative expansion is considered order by order and each order contributes less than the previous. This explains the experimentally observed hierarchy of many-body forces, as forces of higher particle rank appear later in the expansion. At the next-to-next-to-next-to-leading (n^3lo) order, which is the two-body interaction used in all our calculations, already three- and four-body forces are part of the theory. However, the four-body forces are very small at this level.

The chiral interaction is suited to describe low energy processes. The hard scale, where the chiral expansion breaks down, is typically set around 1 GeV, while the interactions elements themselves are only set up to a cutoff below

the hard scale. In the interaction used in this work [8], the cutoff is set at 500 MeV. Thus, the interaction is suitable for ground state energies, low energy excitation spectra and conventional nuclear reactions [5]. At higher energies, QCD becomes perturbative and conventional field theoretic approaches may be used.

2.3 Many-body approximations

In any *ab initio* many-body calculation, there are many different levels of truncations and approximations. Once the nuclear interaction is available, convergence has to be reached at every level, before we can say that we have the final result from a specific interaction. But already in the derivation of the interaction, many approximations have been made. The chiral interaction is expressed as a power series in the ratio between the soft and the hard momentum scale. It is cut off at the level of n^3lo, where both three- and four-nucleon forces are part of the series. Diagrams have to be renormalized to account for divergent integrals and the integrals themselves have to be solved numerically, introducing a slight numerical error. Once these parameters are set, the free coupling constants in the theory are fitted to reproduce nucleon-nucleon scattering phase shifts. The experimental data used also has a varying degree of accuracy, that has to be accounted for in the fitting process. As well as the numerical cutoffs used to solve the Lippmann-Schwinger equation for the two-body system. Finally the matrix elements of the interaction can be produced. For each partial wave, a new set of matrix elements are produced in relative and center-of-mass coordinates. The number of partial waves is unfortunately infinite, so a numerical cutoff has to be introduced also at this level.

In this work, the many-body problem is solved in laboratory coordinates in a discrete harmonic oscillator basis. Single nucleon wave functions define the space of available many-body configurations. This space is called the Hilbert space and represents the space of available wave functions. The size of this space is determined by the number of allowed harmonic oscillator shells. Various intermediate transformations are also performed, each with its own set of approximations, but these present no problems as they are taken to numerical precision.

Once the many-body basis has been defined, the Schrödinger equation can be solved exactly by means of a matrix diagonalization of the many-body Hamiltonian matrix. Unfortunately, this can only be done for light nuclei in relatively small model spaces (see Navrátil et al. [9] for a recent review). Additional approximations are necessary to reach heavier nuclei.

Let us make the previous discussion a bit more concrete, as it is needed to discuss the approximations made in coupled-cluster theory. Given a set of single particle wave functions, we can construct a basis for an A-body Hilbert space $\mathcal{H}$, that consists of all possible Slater determinants that can be constructed from A single particle wave functions. The wave function can be expanded in a linear combination of these Slater determinants

$$|\Psi\rangle \approx |\Phi_0\rangle + \sum_{\substack{i_1\\a_1}} c_{i_1}^{a^1} |\Phi_{i_1}^{a^1}\rangle + \frac{1}{4} \sum_{\substack{i_1,i_2\\a_1,a_2}} c_{i_1 i_2}^{a^1 a_2} |\Phi_{i_1 i_2}^{a^1 a_2}\rangle + \ldots + \frac{1}{(A!)^2} \sum_{\substack{i_1,\ldots,i_n\\a_1,\ldots,a_n}} c_{i_1\ldots i_n}^{a^1\ldots a_n} |\Phi_{i_1\ldots i_n}^{a^1\ldots a_n}\rangle, \quad (2.1)$$

where $|\Phi_0\rangle$ is the reference determinant. $|\Phi_{i_1\ldots i_n}^{a^1\ldots a_n}\rangle$ is the determinant where particles occupying the orbitals labelled $i_1 \ldots i_A$ in the reference determinant has been excited to orbitals labelled $a_1 \ldots a_n$ that are not occupied in the reference state. As is customary in the coupled-cluster literature, orbitals with indices $i, j, k, \ldots$ represent hole states, i.e. single particle states below the Fermi level, while orbitals with indices $a, b, c, \ldots$ represent particle states, i.e. single particle states above the Fermi level. The amplitudes $c_{i_1\ldots i_n}^{a^1\ldots a_n}$ are the probability amplitudes for finding the A-body state in a given configuration.

We can write this in operator form as

$$|\Psi\rangle \approx \hat{\mathrm{C}}|\Phi_0\rangle = \left(\hat{1} + \sum_{n=1}^{A} \hat{\mathrm{C}}_n\right) |\Phi_0\rangle, \quad (2.2)$$

where

$$\hat{\mathrm{C}}_n = \frac{1}{(n!)^2} \sum {}_{a_1,\ldots,a_n}^{i_1,\ldots,i_n} c_{i_1\ldots i_n}^{a^1\ldots a_n} \left\{ a_{a_1}^\dagger \ldots a_{a_n}^\dagger a_{i_n} \ldots a_{i_1} \right\}. \quad (2.3)$$

Here $a_p^\dagger(a_p)$ are creation(annihilation) operators that creates(annihilates) a particle in the orbital labelled p. $\hat{\mathrm{C}}_n$ is called a n-particle n-hole excitation operator, while the curly brackets indicate that the operator product is normal ordered.

Solving the many-body Schrödinger equation in this basis for the unknown c-amplitudes, is called the full configuration interaction method (FCI) in the quantum chemistry literature and is equivalent to the exact diagonalization discussed above. Following this method, approximations are introduced by a truncation of the particle-hole expansion in Eq. (2.1). Such a truncation will in general lead to the inclusion of unwanted unlinked diagrams.

In coupled-cluster theory, we choose a different parametrization of the c-amplitudes, determined by the exponential expansion

$$|\Psi\rangle \approx |\Psi_{CC}\rangle = e^{\hat{\mathrm{T}}}|\Phi_0\rangle, \qquad \hat{\mathrm{T}} = \hat{\mathrm{T}}_1 + \hat{\mathrm{T}}_2 + \ldots + \hat{\mathrm{T}}_A \tag{2.4}$$

where

$$\hat{\mathrm{T}}_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1,i_2,\ldots i_n \\ a_1,a_2,\ldots a_n}} t^{a_1 a_2 \ldots a_n}_{i_1 i_2 \ldots i_n} a^\dagger_{a_1} a^\dagger_{a_2} \ldots a^\dagger_{a_n} a_{i_n} \ldots a_{i_2} a_{i_1}$$

is the n-particle n-hole operator discussed above. Writing the out the Taylor expansion of this operator, reveals the equivalence between the two methods. There is a direct correspondence between the operators $\hat{\mathrm{C}}$ and $\hat{\mathrm{T}}$ in the expansion of the wave function, which is translated into a relation between the individual amplitudes,

$$c^a_i = t^a_i \tag{2.5}$$

$$c^{ab}_{ij} = \frac{1}{2} t^a_i t^b_j + t^{ab}_{ij} \tag{2.6}$$

$$c^{abc}_{ijk} = \frac{1}{6} t^a_i t^b_j t^c_k + t^{ab}_{ij} t^c_k + t^{abc}_{ijk} \tag{2.7}$$

$$\vdots \tag{2.8}$$

Without truncations, the two methods are equivalent, but when truncations are introduced, important differences emerge. When $\hat{\mathrm{C}}$ is truncated, no determinants with higher particle rank than $\hat{\mathrm{C}}$ can be produced. This is not the case when $\hat{\mathrm{T}}$ is truncated, as determinant at all ranks can be produced. The number of degrees of freedom are still identical, but a different manifold is mapped out in the original Hilbert space. As a consequence, no unlinked diagrams appear in coupled-cluster theory.

Different truncations of $\hat{\mathrm{T}}$ defines a hierarchy of coupled-cluster approximations. In nuclear physics, two truncations are used. When $\hat{\mathrm{T}}$ is truncated after 2P-2H amplitudes, the method is called the coupled-cluster singles and doubles (CCSD) approximation. Including triple excitations, by truncation $\hat{\mathrm{T}}$ at the 3P-3H level defines the coupled-cluster singles, doubles and triples (CCSDT) approximation. A peculiar situation arises, because in general CCSD is not accurate enough in nuclear physics applications, while CCSDT is too computationally expensive to be used routinely. Therefore, an additional level of approximation is introduced in Λ-CCSD(T) [10], where the effects of triple excitations are approximated based on only singles and doubles amplitudes. This is an approximation to the approximation, if you will, which has proven to be very accurate and is currently considered state-of-art in coupled-cluster theory for nuclear physics.

Now, the defining equations for the cluster amplitudes can be found in any recent textbook on many-body methods. In Shavitt and Bartlett [11] all relevant equations up to CCSDTQ are listed in full. Once the amplitudes have been defined, the similarity transformed Hamiltonian is defined by

$$\bar{\mathrm{H}} = e^{-\hat{\mathrm{T}}} \hat{\mathrm{H}}_N e^{\hat{\mathrm{T}}}, \tag{2.9}$$

where $\hat{\mathrm{H}}_N$ is the Hamiltonian normal-ordered with respect to the A-body reference state. By diagonalizing this matrix in the proper Hilbert space, approximations to the energy eigenstates of the original Hamiltonian can be found. The Hilbert space is now defined by the standard particle-hole expansion represented by $\hat{\mathrm{C}}$, and an additional level of approximation is introduced by truncating this space. This is called the equation-of-motion coupled-cluster theory (EOM-CC).

Whenever approximations are involved, we want to make sure that despite the approximations introduced, the results are still comparable to the exact solution. But in nuclear physics, this is only half the story. While we must consider the quality of the coupled-cluster approximations by comparing our result to an exact diagonalization in an identical model space, we must simultaneously make sure that the interaction matrix elements we use are a good representation of the original interaction. Now, the quality of the coupled-cluster approximation is basically set. The Λ-CCSD(T) approximation is the best we can do for closed (sub-)shell nuclei. In the diagonalization procedure, we are currently not able to increase the size of the Hilbert space,

due to the large number of single particle wave functions. To refine these approximations, the computational cost needs to be reduced by optimizing the current implementation and an increase in the available computational resources are probably needed. The main challenge is then to make sure that our results are converged with respect to the size of the harmonic oscillator space.

We now introduce two papers, attached to this thesis as paper 1 in appendix A.1 and paper 2 in appendix A.2. These papers introduce an EOM-CC method that is tailored for the calculation of energy states in nuclei that can be described as two nucleons attached to or removed from a closed (sub-)shell nucleus. The first paper compares the results obtained to an exact diagonalization in a small single particle space. The conclusions are discussed in section 2.4. The second paper explores the convergence properties of the method with respect to the size of the single particle space. A discussion of this article can be found in section 2.5. These two articles represent the bulk of the work done in preparation for this thesis.

2.4 Proof of concept

In paper 1 [12], we defined two new methods within coupled-cluster theory, that expanded its reach to nuclei that can be described as two nucleons attached to or removed from a closed (sub-)shell nucleus. Both methods are based on the coupled-cluster singles and doubles (CCSD) approximation to a closed (sub-)shell reference, where a similarity transformation is constructed in a reduced Hilbert space. This results in a non-Hermitian operator labelled $\bar{\mathrm{H}}$, which is often called the similarity transformed Hamiltonian in the literature. To obtain energy levels and eigenstates, $\bar{\mathrm{H}}$ is diagonalized in the space of the Slater determinants that are appropriate for the problem at hand. When two nucleons are added, the method is called two particle attached EOM-CCSD (2PA-EOM-CCSD) and the many-body space is constructed of determinants that have two extra particles compared to the reference determinant. In paper 1, at most 3P-1H determinants were included in the diagonalization procedure. When two nucleons are removed from a reference nucleus, the method is called two particle removed EOM-CCSD (2PR-EOM-CCSD) and only determinants that have two particles less than the reference

are included. At most 1P-3H determinants were included in the current implementation.

There are two reasons why these methods were introduced to nuclear physics. First, as already stated, coupled-cluster theory can be used to study a larger set of nuclei with these methods. Second, and related to the long term goals of the group, is the possibility of constructing effective operators for the use in shell-model calculations. The idea is to use the particle attached EOM-CCSD (PA-EOM-CCSD) and particle removed EOM-CCSD (PR-EOM-CCSD) methods [13–15], which are suited for nuclei where one nucleon is added to or removed from a closed (sub-)shell nucleus, to obtain single particle energies. The methods presented here are then used to obtain an effective interaction in a reduced space by a similar procedure to Shukla et al. [16]. Thus, coupled-cluster theory can be used to study an even larger set of nuclei, also in the heavy mass regime. For this procedure to work, it is crucial that these methods provide accurate approximations to both energy levels and the wave functions. Currently, only energy levels can be obtained as the calculations of other expectation values are more involved. To further evaluate the wave functions, radii, charge distributions, transition probabilities etc. should also be calculated. These properties are more sensitive to changes in the wave function than the energy.

To evaluate the accuracy of the methods, we studied the helium isotopes $3-6$He and compared the approximate results to an exact diagonalization in a very small model space. The quality of the results was mixed. First the PR-EOM-CCSD approximation was unable to accurately describe the ground state of ^{3}He. This was to be expected as the removal of a nucleon from ^{4}He is not considered a good approximation to ^{3}He. This method performs better for heavier nuclei [17, 18].

The main result of the paper, was the quality of the PA-EOM-CCSD and 2PA-EOM-CCSD methods. Both methods were able to provide ground state energies within half a percent of the exact energies for ^{5}He and ^{6}He respectively. ^{6}He, also the 2PA-EOM-CCSD approximation of the first excited $J^\pi = 2^+$ state was within the same level of accuracy.

These nuclei are especially good candidates for the EOM framework. Both nuclei can be described and are viewed as an inert ^{4}He core, interacting with one or two nucleons. ^{4}He is deeply bound, about 20 MeV below the nucleon emission threshold and it has no bound excited states. The alpha cluster

is therefore expected to retain its structure when additional neutrons are added.

2.5 Chasing convergence

One of the main goals of the work leading up to this thesis, has been to do converged calculations of medium mass nuclei like ^{42}Ca and ^{50}Ca, using the "bare" chiral interaction and the 2PA-EOM-CCSD method. From earlier studies [19], it was known that the basis size would have to include at least 17-19 major oscillator shells for convergence in this region. In the previous section, we presented the 2PA-EOM-CCSD method in a basis of Slater determinants, which we will call the uncoupled representation. In the uncoupled representation the largest calculations we performed used a basis size of only five harmonic oscillator shells. This approach was not viable for the large model spaces needed for convergence.

2.5.1 Symmetries

The many-body Hamiltonian has several inherit symmetries. Each of these give rise to a conserved quantum number. While a complete description is beyond the scope of this thesis, a brief discussion of the relevant quantum numbers and the symmetries associated with them, is in order (for details see e.g. Bohr and Mottelson [20]).

The nuclear Hamiltonian is invariant to the familiar space-time transformation. Invariance under translation leads to the conservation of total momentum, invariance under rotation leads to the conservation of the total angular momentum. In addition, the Hamiltonian is invariant with the respect to space inversion, which leads to the conservation of parity. In the Slater determinant basis used in the uncoupled representation, the total parity is a good quantum number. That means that each Slater determinant has a specific parity determined by the orbital momenta of all individual single particle wave functions. The same is also true for the projection of the total angular momentum, which is the sum of all individual projections. The conservation of these quantum numbers was exploited already in the uncoupled representation as the quantum numbers were additive and easy to implement.

The Slater determinant basis does not, in general, have a good total angular momentum. Only the singlet states with zero total angular momentum can be associated with a Slater determinant. A new basis had to be constructed, where each basis state had a specific total angular momentum. This is what we refer to as the coupled representation or the jj-scheme. To accomplish this, a fair bit of angular momentum algebra had to be performed and the resulting algebraic expressions are cluttered with recoupling coefficients, complicated phases and sums over intermediate angular momentum variables. The implementation of these equations is a bug prone operation, and care has to be taken to verify the implementation. The payoff, however, is immense and is one of the major reasons that converged calculations in the medium mass sector were accomplished.

In paper 2, we presented the 2PA-EOM-CCSD method in the coupled representation. The theory presented there as well as the resulting implementation, is the main work of this thesis. For future reference, all algebraic expressions in the coupled representation were listed along with a thorough description of the procedure used to derive them.

2.5.2 Center-of-mass contamination

The nuclear Hamiltonian is invariant under Galilean transformations. This means that the Hamiltonian can be expressed as the sum of an intrinsic part and a center-of-mass part, where the intrinsic Hamiltonian only depends on relative coordinates. When many-body calculations are performed in relative and center-of-mass coordinates, this separation can be treated exactly. For more than a few particles however, this basis is not feasible. Because the explicit anti-symmetrization of the many-body wave functions is more complicated for many particles, the use of this basis for more than four particle is seldom done. In laboratory coordinates, the construction of anti-symmetric wave functions is trivial in the uncoupled representation. While it is more complicated in the coupled representation, the many-body basis consist of only four quasi particles and the coupling procedure is manageable for such systems. The problem, however, is that the final wave function is not guaranteed to factorize into a relative and a center-of-mass part – especially when a truncated space is used as in coupled-cluster theory.

This problem was solved by Hagen et al. [21], where they demonstrated

the approximate factorization of the ground state wave function in the Λ-CCSD(T) approximation. Later, it was also demonstrated for excited states when the procedure was applied to PA-EOM-CCSD states. The factorization was not as good in this case, especially for higher lying excited states.

In paper 2, we demonstrate the factorization of the final wave function also for states calculated with the 2PA-EOM-CCSD approach. Some states, however, like the second $J^\pi = 0^+$ in ^{18}O, shows a large center-of-mass contamination. The other two $J^\pi = 0+$ states factorize approximately with reasonably high accuracy. The factorization was not explored in full, as calculations in larger model spaces have to be performed, but already at the current level there was a major difference between the states that factorize approximately and the ones that do not. We interpret the center-of-mass contamination as an indication that the many-body basis has been truncated prematurely. This can either be in the size of the harmonic oscillator single particle space, the coupled-cluster truncation or the 3P-1H truncation implemented in this work.

2.5.3 Convergence properties

One of the main conclusions reached in paper 2, was that the current implementation was able to calculate converged energies using the "bare" chiral interaction. Both ground state energies and excitation energies were investigated for ^{6}He, ^{6}Li, ^{18}O and ^{18}F, where selected states in both ^{6}Li and ^{6}He were compared to a no-core shell-model (NCSM) calculation [22]. While the ground state energies seemed to converge towards the NCSM result, the excitation energies were consistently overestimated. For some of the excited states, most of the difference can be attributed to the differences between the two calculations. The NCSM results were extrapolated to infinite model spaces and some uncertainties as to the exact parameters used in the interaction exist.

The $J^\pi = 3^+$ excited state in ^{6}Li however, was especially high in energy, about 700 keV compared to the NCSM result. While this is attributed to missing 4P-2H configurations in the EOM diagonalization, we tried to identify if this state displayed some properties that could be used to evaluate the accuracy of the calculation. This would be very useful in heavier nuclei, where exact diagonalization is not possible. We found the center-of-mass contami-

nation of this state especially intriguing, but was unable to reach converged results for this expectation value. The contamination was only a few hundred keV and compared to the spurious center-of-mass states found in the spectrum, this was insignificant. Additional calculations using softer interactions were also performed to speed up convergence, but this contamination did not disappear, as it did for most of the other excited states we looked at. A quantitative analysis of this contamination is something we will have to look at in the future, especially its correlation to the error introduced in the coupled-cluster calculation. There are some obstacles that needs to be overcome before we can go any further. First, the comparison has to be done in a large model space, so that it can be considered complete. This will require substantial computational resources, even if low-momentum interactions are used. Second, the calculation of expectation values in coupled-cluster is not exact. A discretized version of the Hellmann-Feynman theorem is used. A more exact approach would be to calculate the expectation value directly using the final wave function.

Even though the center-of-mass contamination could not be analyzed quantitatively, it still proved a valuable tool. In ^{18}O it was a crucial element in identifying the second $J^\pi = 0^+$ excited state. This state is known to have sizeable contributions from 4P-2H configurations [23] and should therefore not be reproduced in a 2PA-EOM-CCSD calculation where the basis has been truncated at 3P-1H configurations. Our third $J^\pi = 0^+$ state, although the energy was completely converged, had a massive amount of center-of-mass contamination. Under the assumption that center-of-mass contamination suggests an unconverged calculation, we concluded that this state was not converged with respect to the EOM truncation and was an ideal candidate for the experimentally observed second $J^\pi = 0^+$. This was further strengthened in paper 3, where the effects of three-nucleon forces were included. Here our second $J\pi = 0+$ was pushed up in excitation energy to the level of the experimentally observed third $J^\pi = 0^+$.

Three negative parity states also showed a large center-of-mass contamination and were excluded from the final spectrum. In these states, the level of 3P-1H configurations in the final wave function was larger than for the other states. This is natural, as 3P-1H excitations, where a nucleon is excited from the p-shell to the sd-shell, is one of the best ways to create negative parity states. A 2P configuration would have to include an orbital from the pf-shell to create a negative parity state. But larger 3P-1H amplitudes also indicates

the need for additional 4P-2H configurations.

In general, both the ground and excited states in ^{18}O and ^{18}F, showed a reasonable level of convergence using 17 major oscillator shells. This requires about 300 coupled single particle wave functions and resulted in up to 300 million coupled configurations($J^\pi = 5^+$ in ^{18}F) at the 3P-1H level, which determines the dimensionality of the matrix to be diagonalized.

In papers 3 and 4, the 2PA-EOM-CCSD method was used to calculate the binding energy and excitation energies of more neutron rich nuclei. While the rate of convergence with respect to the size of the model space was reduced, we were still able to perform converged calculations of both ^{26}O and ^{56}Ca. The latter required 21 harmonic oscillator shells before the ground state energy was converged and is the largest model space attempted with the current implementation. As more neutrons are added, the neutron drip line is getting closer and the isotopes are more weakly bound. A closer proximity to the nucleon emission threshold requires a larger model space when the harmonic oscillator basis is used. As only bound states are allowed by this basis, a large number of single particle wave functions are needed to account for the effect of the continuum. As we shall see in the next section, a different basis is more appropriate for such systems.

An additional point can be made about neutron rich systems in relation to the 2PA-EOM-CCSD method. In paper 4 we also calculated the excitation spectra of ^{50}Ti, ^{54}Ti and ^{56}Ti. These were obtained by adding two protons in the $f_{7/2}$ orbital. This orbital and those immediately above, were already fully occupied by neutrons in these systems. Compared to the respective Calcium isobars, the results were not as good for these nuclei. This can be related to the proton-neutron interaction between protons in the $f_{7/2}$ orbital and neutrons in the orbitals $f_{7/2}$, $p_{3/2}$ etc. These are above the level of occupation in proton orbitals, but below that of neutron orbitals. The interaction between nucleons in these orbitals are now particle-hole interactions and not particle-particle interactions as they would be in symmetric nuclei. The effect is that additional levels of particle-hole correlations are needed when protons are added to neutron rich reference states. It is probable that this is also the case when adding a proton neutron pair. The final wave functions of the titanium isotopes showed a significantly larger 3P-1H content, than their corresponding calcium isobars.

Chapter 3

Applications

Until now, the main focus of this thesis has been the development of the 2PA-EOM-CC method as well as its accuracy and convergence properties. We have shown that this method is suitable for calculating binding energies and the excitation energies of low lying states with simple structure. However, it has been assumed that all states are bound, which are the only type of states allowed by the harmonic oscillator single particle basis. In addition, it has been assumed that the nuclear Hamiltonian contains only two-body interactions. None of these assumptions survive comparison with experimental data.

3.1 Three-nucleon forces

It has been known for some time that the inclusion of three-nucleon forces (3NF) is necessary for a quantitative description of nuclei. In 2001, Pieper and Wiringa [24] showed explicitly that for light p-shell nuclei, nuclear properties can be accurately described starting from NN and 3NFs only.

For many-body methods based on a finite basis expansion, the inclusion of 3NFs is a formidable task. While the number of two-body matrix elements scale as $O(n^4)$, the number of three-body matrix elements scale as $O(n^6)$, where n is the number of single particle basis states. As we saw in section 2.5, approximately 300 single particle states were used for a converged cal-

culation of the binding energy of ^{18}O, using the bare n^{3}lo interaction. Thus, the number of three-body matrix elements for this calculation would be five orders of magnitude larger than the number of two-body matrix elements. The storage of matrix elements are already a limiting factor in many-body calculations, so a full treatment of 3NFs is not possible. We highlight two strategies to deal with this problem.

3.1.1 Renormalized three-nucleon forces

The major reason why a large model space is needed for a converged calculation, is because the interaction is hard. This means that it contains high momentum components that will slow the rate of convergence. A softer interaction where the short range components have been removed, will reduce the number of matrix elements needed. This is the approach taken in recent no-core shell-model calculations, where the similarity renormalization group (SRG) method [25] has been used to create effective low-momentum interactions.

There is a potential problem with this approach, that has yet to be resolved. The renormalization procedure itself induces many-body operators of higher rank than the original. This means that if the original operator was a two-body operator, the effective operator will contain three-body parts and higher. If the induced many-body operators are small, they can be safely neglected. If not, the final result will have a significant model dependence. This is illustrated in Roth et al. [26], where they conclude that when starting from a Hamiltonian that includes 3NFs, the SRG approach will induce sizeable four-nucleon forces.

These conclusions were drawn by extrapolating the result using effective interactions with different values of the SRG model parameter. The extrapolated values differed substantially. Now, this calculation can be criticized for using a fixed $\hbar\omega$ value in their calculations. If the $\hbar\omega$ dependence is different for the different values of the SRG model parameter, the extrapolations done in Roth et al. [26] will not describe the complete picture. This matter is not yet resolved and a more detailed analysis will hopefully enlighten the situation.

3.1.2 Density-dependent three-nucleon forces

The inclusion of 3NFs in coupled-cluster theory is faced with a different problem. A full inclusion using the CCSDT approximation, will require close to a thousand new diagrams to be added. This is a formidable task and will probably not be attempted any time soon.

In Hagen et al. [27], coupled-cluster theory for three-body Hamiltonians was presented at the CCSD level in the uncoupled scheme. A detailed analysis of the contribution from the 3NFs was performed for ^{4}He. They showed that by including only the density-dependent zero-, one- and two-body parts of the normal ordered Hamiltonian used in coupled-cluster theory, most of the effects of the original 3NFs were accounted for. The residual three-body Hamiltonian accounted for less than a thousandth of the total binding energy. It must be said, that these calculations were done in very small model spaces with soft low-momentum interactions. The authors warn that this result might be due to the softness of the effective interaction used in the calculations. A more recent result, not yet published is presented in Roth et al. [28], where the same approach is used for heavier nuclei, show the same result. The residual interaction contributes very little to the total energies, but also here, soft effective interactions were used in the analysis.

But even using this approach, the full set of three-body matrix elements have to be stored and used to calculate the density dependent parts. A different approach was proposed by Holt et al. [29]. They proposed an effective three-body interaction based on chiral perturbation theory at next-to-next-to leading order. By integrating one nucleon line on all three-body diagrams at this level up to the Fermi momentum, this line was closed creating an effective two-body diagram. This procedure is designed for symmetric nuclear matter, but we wanted to investigate how this relatively simple effective interaction performed when used in finite nuclei. The result has been two papers [30, 31], attached to this thesis as paper 3 in appendix A.3 and paper 4 in appendix A.4, where this interaction is used on the oxygen and the calcium chain of isotopes.

3.2 Nuclei as open quantum systems

When moving away from the valley of stability, it becomes evident that the nuclei are not completely isolated systems. Weakly bound nuclei have ground states very close to their nucleon emission thresholds, while unbound nuclei might have resonant states that are detectable in modern experiments. A complete description of nuclei, would have to take this openness into consideration.

In the Gamow shell model [32], bound, resonant and continuum states are all accounted for on equal grounds by using the Berggren completeness relations [33]. The resulting basis can be used in standard many-body calculations by transforming the basis and matrix elements to a discrete basis in laboratory coordinates, as has been done in Hagen et al. [34, 35]. The entire coupled-cluster machinery can then be used, with a more correct treatment of continuum degrees of freedom, resulting in better results for nuclei and states close to the nucleon emission threshold. When resonances are to be included, a complex valued basis has to be used. The The inclusion of resonances in particle attached or removed methods presents some issues, as the resonance is calculated with respect to the wrong threshold. This is the direct consequence of the treatment of the center-of-mass energy in the original Hamiltonian.

In both papers 3 and 4, the effects of continuum degrees of freedom were shown to be crucial for the description of neutron rich nuclei.

3.3 Oxygen

The oxygen isotopes are particularly interesting nuclei. Especially the neutron rich isotopes where new magic numbers have been established. It is also the heaviest element with an experimentally established drip line. Earlier studies have shown the need for both a correct inclusion of continuum degrees of freedom [36, 37] and that 3NFs were crucial to explain experimental data [38]. None has performed a complete calculation for the oxygen isotopes treating both continuum degrees of freedom and 3NFs simultaneously. This is what we set out to do in Hagen et al. [30] attached to this thesis as paper 3 in appendix A.3.

3.3.1 The oxygen drip line

Oxygen is the heaviest nuclei for which the neutron drip line is experimentally established. But the theoretical prediction of this drip line has not been easy. In Otsuka et al. [38] it was shown that the inclusion of the effects of 3NFs are necessary for establishing the correct drip line nucleus. Earlier studies, including coupled-cluster [37], where only NN interactions were used, were not able to do do this. Using the density-dependent effective interaction described earlier to approximate the 3NFs from chiral perturbation theory, we were able to reproduce the drip line in the oxygen isotopes. This was considered clear evidence that this interaction includes important aspects of the 3NFs. Fig. 1 in Hagen et al. [30] clearly show that 3NFs are necessary for establishing the correct drip line.

3.3.2 Magic numbers

The nuclear shell-model [39] is the current paradigm for our understanding of nuclear structure. In this model, the magic numbers are particularly important, because they denote especially stable numbers of protons and neutrons. The so-called doubly magic nuclei have a magic number of both protons and neutrons. The magic numbers where observed along the valley of stability and were explained theoretically by a mean field in addition to a strong spin-orbit interaction. But as the neutron to proton ratio change, so does the magic numbers. In the oxygen chain, new doubly magic nuclei have been established at ^{22}O and ^{24}O [40–42], making neutron numbers $N = 14$ and $N = 16$ magic. The strongest experimental evidence for doubly magic structure, is a high excitation energy of the first excited state compared to that of neighbouring nuclei, due to the large energy gap up to the next available orbital.

We find this high lying first excited state both in ^{22}O and ^{24}O, but the inclusion of 3NFs is crucial for both results. In ^{24}O the first excited $J^\pi = 2^+$ is in the continuum, so continuum degrees of freedom are important for this state. However, we did not investigate the specific effect of the continuum degrees of freedom for this state.

3.3.3 Predictions

The ultimate goal of nuclear many-body theory is to be fully predictive. In paper 3 attached to this thesis in appendix A.3, we make several predictions of observables not yet measured experimentally. The ground state of ^{28}O, a resonance, is predicted to be unbound with respect to ^{24}O by about 4 MeV with a resonant width of about 1 MeV. Without 3NFs this state would be bound compared to ^{24}O and would constitute the oxygen drip line [37]. Without continuum couplings, the energy would be much closer to that of ^{24}O.

We also predict three narrow resonances near the unknown experimental state at about 7.5 MeV in ^{24}O [43]. This supports Hoffman et al. [43], where they speculate that this resonance is a superposition of narrow resonances with $J^\pi = 1^+$ to 4^+. We however, find the $J^\pi = 1^+$ state at significantly higher energy and shorter lifetime. Both 3NFs and continuum degrees of freedom were again crucial for finding these states at the reported values.

3.4 Calcium

In the oxygen isotopes, the inclusion of 3NFs was crucial for making ^{24}O doubly magic and a drip line nucleus. In the calcium isotopes the drip line is an unsettled topic. The heaviest isotope where mass measurement has been done is ^{52}Ca [44, 45], while energy-functional [46] and mass-models [47, 48] predict the drip line to be around ^{70}Ca, leaving lots of room for predictions. In addition, mean-field calculations [47, 48] predict that the single particle states above ^{60}Ca are very closely spaced. As a result, the nuclei in this region might be very deformed, making a coupled-cluster approach difficult due to missing correlations. The evolution of shell structure in this region is particularly interesting and might hold similar surprises as the new magic neutron numbers found in the oxygen chain.

In paper 4, attached to this thesis in appendix A.4, we focused on the description of shell structure in neutron rich calcium isotopes in the $A = 50$–60 region, including both 3NFs and continuum degrees of freedom.

3.4.1 Shell closure

Experimentally, both ^{40}Ca and ^{48}Ca are well established doubly magic nuclei. But two-body forces alone does not yield a magic neutron number at $N = 28$. Again, the inclusion of 3NFs is necessary, as shown by Holt et al. [49]. At neutron number $N = 32$ a so-called sub-shell closure is well established in chromium, titanium and calcium [50–53]. At neutron number $N = 34$ however, no sub-shell closure is seen in either chromium or titanium [54–56], but the matter is still unsettled in calcium [57]. Theoretical studies [49, 58–60] predict everything from no shell gap to a large shell gap indicative of a major shell closure.

In the coupled-cluster calculations presented in paper 4, our results confirmed those of Holt et al. [49] – that the inclusion of 3NFs is needed for ^{48}Ca to be doubly magic and that the neutron number $N = 32$ generates a sub-shell closure in ^{52}Ca. One of our main results was the sub-shell closure of ^{54}Ca as well. The first excited $J^\pi = 2^+$ state in ^{54}Ca, was very similar in energy to the first excited state in ^{52}Ca. In addition the $J^\pi = 4^+$ to 2^+ ratios were similar.

3.4.2 Drip line

As can be seen from Fig. 1 in paper 4, coupled-cluster calculations using the density-dependent effective 3NF derived by Holt et al. [29], places the neutron drip line in the calcium isotopes to be between ^{56}Ca and ^{60}Ca. We place the ^{60}Ca slightly unbound compared to ^{56}Ca, but missing many-body correlations might be more important for the description of ^{60}Ca, than for ^{56}Ca. This can result in additional binding in ^{60}Ca, so a definite conclusion cannot be drawn on this subject.

But something interesting happens to the single particle states in this region. The first orbitals above ^{60}Ca, where the neutron pf-shell is filled, changes order in our calculation compared to the shell model picture. In the shell-model, the first three single particle states above the pf-shell is the $g_{9/2}$, the $d_{5/2}$ and the $s_{1/2}$ orbitals. In our calculations, the $J^\pi = 5/2^+$ state drops below the $J^\pi = 9/2^+$ state in ^{53}Ca, ^{55}Ca and ^{61}Ca. Also in ^{61}Ca, the $J^\pi = 1/2^+$ state drops even lower than $J^\pi = 5/2^+$. In addition, the ground state of ^{62}Ca, is completely dominated by $(s_{1/2})^2$ configurations. This effect is

all due to the correct treatment of the scattering continuum. Without these additional degrees of freedom, our calculations reproduce the shell-model ordering.

3.5 The complete picture

There are two major conclusion that I want two highlight from this chapter. First, a complete description of nuclei is not possible without the inclusion of three-nucleon forces and the correct treatment of the scattering continuum. Without these two elements, important structural information like shell closure, the location of the drip line and even the ordering of single particle states will not be reproduced. A correct treatment of the scattering continuum will also facilitate a more unified approach to both structure and reactions.

Second, and absolutely paramount to coupled-cluster theory, the effects of three-nucleon forces can be approximated by density-dependent effective interactions at the two-body level. It must be noted that the interaction we have used is based on a very crude approach and additional refinements of this interaction will hopefully make this approximation even more useful in practical calculations.

Chapter 4

Concluding remarks

The introduction of the 2PA-EOM-CCSD method to nuclear physics has been very successful. Even though a truncation has been introduced where at most 3P-1H configurations are allowed on top of a coupled-cluster reference state, the quality of our results are quite high. Of course, additional refinements must be introduced to allow even higher accuracy, but many of the results provided can be used quantitatively even now. The binding energies were especially close to a full diagonalization using the same interaction, even though an extrapolation was done after the diagonalization.

If we take a moment and look to the future, one of the many promising uses of this method, is the construction of effective operators for shell-model calculations. Within the coupled-cluster framework, a completely microscopic shell-model input can be calculated. The PA-EOM-CCSD method can provide effective one-body operators and single particle energies, while this method is used for the effective two-body operators. But this requires that we are able to reproduce all relevant states in an effective model space, to a high degree of accuracy. For heavier nuclei, significant improvements have to be made to allow the converged calculations of states with a large total angular momentum. While the *sd*-shell allow a maximum total angular momentum of five, including the pf-shell bring this up to seven. As an effect the number of possible configurations at the 3P-1H level quadruples within identical single particle spaces. One solution might be to reduce the many-body space even further by introducing a different cutoff in the single particle space for 3P-1H configurations than for 2P configurations, similar

to the active space methods presented in Gour et al. [61]. Physically this can be justified as the excitations around the Fermi level is thought to be the most important. This might also be a possible way to introduce 4P-2H configurations. This is an important contribution to excitations in nuclei, because it can be viewed as an excited alpha cluster. Excitations to highly excited states seem even more improbable for such excitations.

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Appendix A

Attachments

A.1 Paper 1: Towards open-shell nuclei with coupled-cluster theory

A.2 Paper 2: Spherical coupled-cluster theory for open-shell nuclei

A.3 Paper 3: Continuum effects and three-nucleon forces in neutron-rich oxygen isotopes

A.4 Paper 4: Evolution of shell structure in neutron-rich calcium isotopes