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# Nuclear Structure Calculations with Coupled Cluster Methods from Quantum Chemistry

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We present several coupled-cluster calculations of ground and excited states of $^4$He and $^{16}$O employing methods from quantum chemistry. A comparison of coupled cluster results with the results of exact diagonalization of the hamiltonian in the same model space and other truncated shell-model calculations shows that the quantum chemistry inspired coupled cluster approximations provide an excellent description of ground and excited states of nuclei, with much less computational effort than traditional large-scale shell-model approaches. Unless truncations are made, for nuclei like $^{16}$O, full-fledged shell-model calculations with four or more major shells are not possible. However, these and even larger systems can be studied with the coupled cluster methods due to the polynomial rather than factorial scaling inherent in standard shell-model studies. This makes the coupled cluster approaches, developed in quantum chemistry, viable methods for describing weakly bound systems of interest for future nuclear facilities.

## 1. INTRODUCTION

Physical properties, such as masses and life-times, of very short-lived, and hence very rare, nuclei are important ingredients that determine element production mechanisms in the universe. Given that present and future nuclear structure research facilities will open significant territory into regions of medium-mass and heavier nuclei, it becomes important to investigate theoretical methods that will allow for a description of medium-

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mass systems that are involved in such element production. Such systems pose significant challenges to existing nuclear structure models, especially since many of these nuclei will be unstable and short-lived. How to deal with weakly bound systems and coupling to resonant states is an unsettled problem in nuclear spectroscopy. Furthermore, existing shell-model methods are limited to very few major shells and/or number of active particles. Similar constraints apply to ab initio Monte Carlo approaches. It is thus critical to develop new computational techniques which not only can handle several major shells but also perform ab initio calculations starting with the free nucleon-nucleon interaction in many-body systems larger than for example $^{40}$Ca.

In this work we focus on coupled cluster methods in our discussion of systems involving many single-particle degrees of freedom. The ab initio coupled-cluster theory is a particularly promising candidate for such endeavors due to its enormous success in quantum chemistry. Based on the experience from quantum chemistry, where coupled cluster methods can be applied to large molecular systems with more than hundred correlated electrons, we anticipate that quantum chemistry inspired coupled cluster approaches will enable accurate studies of ground and excited states of nuclei with dimensionalities beyond the capability of present shell-model approaches, with a much smaller numerical effort. Even though the shell-model combined with appropriate effective interactions offers in general a very good description of several stable and even weakly bound nuclei, the increasing single-particle level density of weakly bound systems makes it imperative to identify and investigate methods that will extend to unstable systems, systems whose dimensionality is beyond reach for present shell-model studies, typically limited today to systems with at most $\sim 10^9$ basis states.

In this contribution we present results of coupled cluster calculations for ground and excited states of $^4$He and $^{16}$O. Where possible, we compare these calculations with exact diagonalization from shell-model studies within the same model spaces and with the same interaction. This serves to underline the reliability of the coupled cluster method in the nuclear many-body problem. The coupled cluster calculations are rather inexpensive compared with the shell-model approach, a feature which is very useful if one wants to include additional degrees of freedom such as more single particle levels. We end this contribution with a discussion of future projects.

## 2. COUPLED CLUSTER APPROACH TO NUCLEI

Coupled cluster theory originated in nuclear physics [1] around 1960. Early studies in the seventies [2] probed ground-state properties in limited spaces with free nucleon-nucleon interactions available at the time. The subject was revisited only recently by Bishop *et al.* [3], for further theoretical development, and by Mihaila and Heisenberg [4], for coupled cluster calculations using realistic two- and three-nucleon bare interactions and expansions in the inverse particle-hole energy spacings. However, much of the impressive development in coupled cluster theory made in quantum chemistry in the last 20-25 years [5–10], after the introduction of coupled-cluster theory and diagrammatic methods to chemistry, by Čížek and Paldus [7,8], still awaits applications to the nuclear many-body problem.

Many solid theoretical reasons exist that motivate a pursuit of coupled-cluster methods.

First of all, the method is fully microscopic and is capable of systematic and hierarchical improvements. Indeed, when one expands the cluster operator in coupled-cluster theory to all $A$ particles in the system, one exactly produces the fully-correlated many-body wave function of the system. The only input that the method requires is the nucleon-nucleon interaction. The method may also be extended to higher-order interactions such as the three-nucleon interaction. Second, in its standard formulation, the method is size extensive meaning that only linked diagrams appear in the computation of the energy (the expectation value of the Hamiltonian) and amplitude equations. It is well-known in for example quantum chemistry that all shell model calculations that use particle-hole truncation schemes actually suffer from the inclusion of disconnected diagrams in computations of the energy. Third, coupled-cluster theory is also size consistent which means that the energy of two non-interacting fragments computed separately is the same as that computed for both fragments simultaneously. In chemistry, where the study of reactive and non-reactive collisions of molecules are very important, this is a crucial property not available in the truncated shell model (named limited configuration interaction in chemistry). Fourth, while the theory is not variational, it does not have a bound, the energy behaves as a variational quantity in most instances. Finally, from a computational point of view, the practical implementation of coupled cluster theory is amenable to parallel computing.

The basic idea of coupled-cluster theory is that the correlated many-body wave function $\mid \Psi\rangle$ may be obtained by application of a cluster operator, $T$, such that $|\Psi\rangle = \exp(T)\,|\Phi\rangle$ where $\Phi$ is a reference Slater determinant chosen as a convenient starting point. For example, we use the filled $0s$ state as the reference determinant for $^4$He.

The cluster operator $T$ is given by $T = T_1 + T_2 + \cdots T_A$ and represents various $n$-particle-$n$-hole ($n$p-$n$h) excitation amplitudes such as

$$T_1 = \sum_{a>\varepsilon_f, i\leq\varepsilon_f} t_a^i a_a^\dagger a_i \qquad T_2 = \frac{1}{4}\sum_{i,j\leq\varepsilon_f; ab>\varepsilon_f} t_{ab}^{ij} a_a^\dagger a_b^\dagger a_j a_i, \tag{1}$$

and higher-order terms for $T_3$ to $T_A$. The basic approximation is obtained by truncating the many-body expansion of $T$ at the $2p-2h$ cluster component $T_2$. This is commonly referred to in the literature as coupled-cluster singles and doubles (CCSD). We compute the ground-state energy from

$$E_0 = \langle\Phi|\bar{H}^{(\mathrm{CCSD})}|\Phi\rangle, \tag{2}$$

where $\bar{H}^{(\mathrm{CCSD})} = \exp(-T)\,H\exp(T)$ is the coupled cluster similarity transformed hamiltonian. In CCSD we set $T = T_1 + T_2$. To derive the CCSD or other coupled cluster approaches, we use the diagrammatic approach. In order to obtain the computationally efficient algorithms, which lead to the lowest operation count and memory requirements, it is better to use the idea of recursively generated intermediates and diagram factorization [6]. The resulting equations can be cast into a computationally efficient form, where diagrams representing intermediates multiply diagrams representing cluster operators. The resulting equations can be solved using efficient iterative algorithms, see for example Refs. [6,11].

### 2.1. Effective Two-body Hamiltonian

In shell-model studies of various nuclear mass regions, the common approach in deriving an effective interaction for the shell-model has been to start with various perturbative many-body approaches, for recent reviews see Refs. [12,13].

The starting point for the derivation of such an effective interaction is normally a bare nucleon-nucleon interaction fitted to reproduce low-energy scattering data. However, since this interaction has a strongly repulsive core at short internucleon distances, one needs to renormalize the short-range part in order to render it suitable for an eventual perturbative treatment. To do that, one sums normally the class of two-body particle-particle ladder diagrams to infinite order. This yields a new and renormalized interaction, the so-called reaction matrix $G$ or just the $G$-matrix. It is however energy dependent, as is the scattering matrix $T$. It differs from the free scattering matrix $T$ by the introduction of a Pauli operator accounting for a specific nuclear medium. The $G$-matrix is in turn used in a perturbative many-body scheme including higher-order corrections, such as core-polarization terms. Such an effective interaction has been a very succesful starting point for shell-model studies. To derive effective interactions within the framework of many-body perturbation theory is however hard to expand upon in a systematic manner by including for example three-body diagrams. In addition, there are no clear signs of convergence, even in terms of a weak interaction such as the $G$-matrix. Even in atomic and molecular physics, many-body perturbative methods are not much favoured any longer, see for example Ref. [14] for a critical discussion. The lessons from atomic and molecular many-body systems clearly point to the need of non-perturbative resummation techniques of large classes of diagrams.

This is one of the main reasons for why we have chosen to focus on the coupled cluster method. However, coupled cluster calculations of nuclei, see Refs. [2–4] have typically started with the bare nucleon-nucleon interaction. As mentioned above, to renormalize this interaction one needs a very large set of single-particle states. The latter makes our use of quantum chemistry algorithms of little practical use if we were to start with the bare interaction.

To circumvent this problem, we define an effective two-body hamiltonian taylored to a specific model space. The single-particle states defining the model space, are in turn used as the basis for our coupled cluster calculations. Here we employ a $G$-matrix defined with a so-called no-core Pauli operator, with the harmonic oscillator defining our single-particle basis. Our model space is then a function of various harmonic oscillator shells. The two-body states defining the $G$-matrix model space are shown in Fig. 1, with $n_3$ representing a large number, at least eight to ten major oscillator shells. The single-particle states labeled by $n_3$ represent then the last orbit of the model space $P$, This so-called no-core model space is used in our definitions of model spaces for the resummations of many-body terms in coupled cluster theory. In Fig. 1 the two-body state $|(pq)JT_Z\rangle$ does not belong to the model space and is included in the computation of the $G$-matrix. Similarly, $|(p\gamma)JT_Z\rangle$ and $|(\delta q)JT_Z\rangle$ also enter the definition of $Q$ whereas $|(\delta\gamma)JT_Z\rangle$ is not included in the computation of $G$. This means that correlations not defined in the $G$-matrix need to be computed by other non-perturbative resummations or many-body schemes. This is where the coupled-cluster scheme enters.

With the $G$-matrix model space $P$ of Fig. 1 we can now define an appropriate space

for coupled-cluster calculations where correlations not included in the $G$-matrix are to be generated. This model space is defined in Fig. 2, where the label $n_p$ represents the same single-particle orbit as $n_3$ in Fig. 1.

The $G$-matrix computed according to Fig. 1 does not reflect a specific nucleus and thereby single-particle orbits which define the uncorrelated Slater determinant. For a nucleus like $^4$He the $0s_{1/2}$ orbit is fully occupied and defines thereby single-hole states. These are labeled by $n_\alpha$ in Fig. 2. For $^{16}$O the corresponding hole states are represented by the orbits $0s_{1/2}$, $0p_{3/2}$ and $0p_{1/2}$. With this caveat we can then generate correlations not included in the $G$-matrix and perform resummations of larger classes of diagrams.

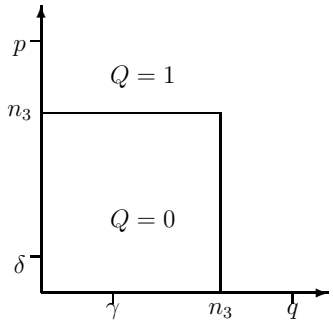


Figure 1. Definition of the exclusion operator $Q$ used to compute the $G$-matrix for large spaces.

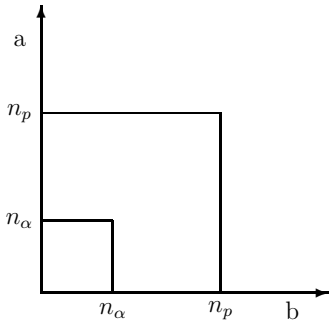


Figure 2. Definition of particle and hole states for coupled-cluster calculations in large spaces. The orbit represented by $n_\alpha$ stands for the last hole state whereas $n_p$ represents the last particle orbit included in the $G$-matrix model space. The hole states define the Fermi energy.

The effective two-body hamiltonian defined by this $G$-matrix depends then on the size of the model space, viz. the number of harmonic oscillator shells, the oscillator parameter and the starting energy of the $G$-matrix. Folded-diagrams are also included in order to reduce the starting energy dependence, see Refs. [11,12] for more details. However, since we are using a two-body interaction in a many-body environment, the starting energy dependence may vary from one many-body system to another. A critical discussion of this dependence is given in the next subsection.

One possible way to avoid such an energy dependence is to use a similarity transformed hamiltonian, where one diagonalizes the two-body problem in a large harmonic oscillator basis, big enough to reproduce the binding energy of the deuteron. Through a similarity transformation one can project this problem onto a smaller space, consisting of some

few oscillator shells and obtain an effective two-body interaction pertaining to this space. This follows the philosophy adopted in the so-called 'no-core' shell-model calculations of Ref. [15]. This interaction is energy independent and depends only on the choice of the model space. The effect of the this approach will be studied in future works.

Finally, we approximately removed the center-of-mass motion by subtracting the kinetic energy of the system from the Hamiltonian, see Ref. [11] for further details.

### 2.2. Ground State Features

In our coupled-cluster study of Ref. [11], we performed calculations of the $^4$He and the $^{16}$O ground state for up to seven major oscillator shells as a function of $\hbar\omega$. We applied the center-of-mass correction described above. We demonstrate how this procedure behaves when one solves the CCSD equations in Fig. 3 for $^4$He as a function of increasing model space for different values of the starting energy. While starting energies larger than $-10$ MeV are affected by the growing model space (due to the proximity of the deuteron pole), for starting energies below about $-20$ MeV results change by less than 1% as we increase the model space from $N = 6$ to $N = 7$. The ground-state energy using the interaction model Idaho-A was quoted as -27.40 MeV by Navratil and Ormand in Ref. [16]. At the level of CCSD, a result of around $-26.5$ MeV would be desired, thus leaving room for additional binding coming from triples correlations. We obtain this result for a starting energy of approximately $-30.0$ MeV. Such a value for the starting energy would also be in good agreement with the fact that it is meant, within the context of perturbative many-body methods, to represent the unperturbed energy of two nucleons. A better approach is most likely the use of a similarity transformed effective interaction, as done by the no-core collaboration, see for example Ref. [15].

In our calculations we have not included the contribution from the Coulomb interaction.

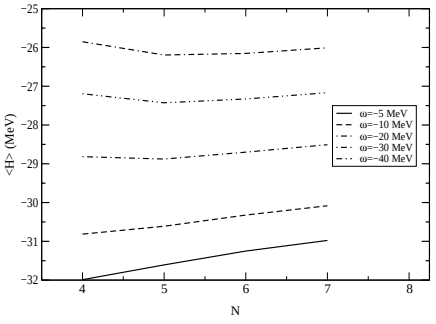


Figure 3. The total energy of $^4$He as a function of increasing model-space size, for different values of the starting energy.

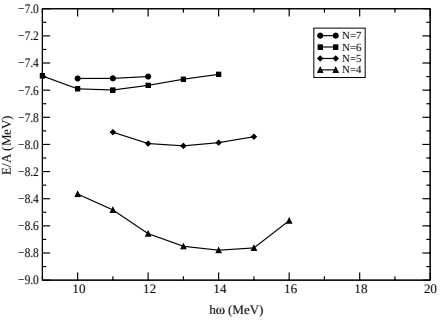


Figure 4. Dependence of the ground-state energy of $^{16}$O on $\hbar\omega$ as a function of increasing model space.

We performed also calculations of the $^{16}$O ground state for up to seven major oscillator shells as a function of $\hbar\omega$. Fig. 4 indicates the level of convergence of the energy per

particle for $N = 4, 5, 6, 7$ shells. The experimental value resides at 7.98 MeV per particle. This calculation is practically converged. By seven oscillator shells, the $\hbar\omega$ dependence becomes rather minimal and we find a ground-state binding energy of 7.52 MeV per particle in oxygen using the Idaho-A potential. Since the Coulomb interaction should give approximately 0.7 MeV/A of repulsion, and is not included in this calculation, we actually obtain approximately 6.80 MeV of nuclear binding in the 7 major shell calculation which is somewhat above the experimental value. We note that the entire procedure ($G$-matrix plus CCSD) tends to approach from below converged solutions. We have recently performed calculations with eight major shells, and the results are practically converged.

In Ref. [17] we considered chemistry inspired noniterative corrections due to $T_3$ clusters (triples in quantum chemistry) to the ground state energy. The presented results are obtained for a model space consisting of four major oscillator shells. Such a space allows us to make comparisons with truncated shell-model (SM) calculations. Table 1 shows the total ground-state energy values obtained with the CCSD and one of the triples-correction approaches (labeled CR-CCSD(T) [9,10,18,19] in the table). Slightly differing triples-corrections yield similar corrections to the CCSD energy. The coupled cluster methods recover the bulk of the correlation effects, producing the results of the SM-SDTQ, or better, quality. SM-SDTQ stands for the expensive shell-model (SM) diagonalization in a huge space spanned by the reference and all singly (S), doubly (D), triply (T), and quadruply (Q) excited determinants. To understand this result, we note that the CCSD $T_1$ and $T_2$ amplitudes are similar in order of magnitude, indeed for an oscillator basis, both $T_1$ and $T_2$ contribute to the first-order MBPT wave function. Thus, the $T_1T_2$ *disconnected* triples are large, much larger than the $T_3$ *connected* triples, and the difference between the SM-SDT (SM singles, doubles, and triples) and SM-SD energies is mostly due to $T_1T_2$.The small $T_3$ effects, as estimated by CR-CCSD(T), are consistent with the SM diagonalization calculations. If the $T_3$ corrections were large, we would observe a significant lowering of the CCSD energy, far below the SM-SDTQ result. Moreover, the CCSD and CR-CCSD(T) methods bring the nonnegligible higher-than-quadruple excitations, such as $T_1^3T_2$, $T_1T_2^2$, and $T_2^3$, which are not present in SM-SDTQ. It is, therefore, quite likely that the CR-CCSD(T) results are very close to the results of the exact diagonalization, which cannot be performed. These results indicate that the bulk of the correlation energy within a

Table 1
The ground-state energy of $^{16}$O calculated using various coupled cluster methods and oscillator basis states. The model space consists of four oscillator shells

| Method | Energy |
|---|---|
| CCSD | -139.310 |
| CR-CCSD(T) | -139.467 |
| SM-SD | -131.887 |
| SM-SDT | -135.489 |
| SM-SDTQ | -138.387 |

nucleus can be obtained by solving the CCSD equations. This gives us confidence that

we should pursue this method in open shell systems and in calculations for excited states.

### 2.3. Excited States

We have recently [17] performed excited state calculations on $^4$He using the EOM-CCSD (equation of motion CCSD) method. For the excited states $|\Psi_K\rangle$ and energies $E_K^{(\mathrm{CCSD})}$ ($K > 0$), we apply the EOMCCSD ("equation of motion CCSD") approximation [20,21] (equivalent to the response CCSD method [22]), in which $|\Psi_K\rangle = R_K^{(\mathrm{CCSD})} \exp(T^{(\mathrm{CCSD})})|\Phi\rangle$. Here $R_K^{(\mathrm{CCSD})} = R_0 + R_1 + R_2$ is a sum of the reference ($R_0$), 1p-1h ($R_1$), and 2p-2h ($R_2$) components obtained by diagonalizing $\bar{H}^{(\mathrm{CCSD})}$ in the same space of singly and doubly excited determinants $|\Phi_i^a\rangle$ and $|\Phi_{ij}^{ab}\rangle$ as used in the ground-state CCSD calculations. As for the ground state, these calculations may also be corrected in a non-iterative fashion using the excited state extension of the completely renormalized (CR-CCSD(T)) approach, see Refs. [9,19,23]. The low-lying $J = 1$ state most likely results from the center-of-mass contamination which we have removed only from the ground state. The $J = 0$ and $J = 2$ states calculated using EOMCCSD and CR-CCSD(T) are in excellent agreement with the results from the shell-model diagonalizations in the same model space. We have recently also computed excited states in $^{16}$O, with a particular emphasis on the first $3_1^-$ state, which is known to be of a 1p-1h nature. Our results based on the EOMCCSD method yields 13.57 MeV for five shells and 12.98 MeV for six shells, to be compared with the experimental value of 6.13 MeV. We expect that with seven shells and the inclusion of triples to get closer to the experimental value. For states like this and for two-body interactions it is well known in quantum chemistry that EOMCCSD is a very accurate approach, producing excitation energies within few per cent of the exact values. Thus, we will be able to predict the result corresponding to an Idaho-A potential that we used in these calculations once we complete our work for the 7 shells and extrapolate the energies to the complete basis set limit. These results will be presented elsewhere, see Ref. [24]. There results for rms radii ($r_{\mathrm{rms}}$) and form factors are also discussed. Here we limit ourselves to note that for $^{16}$O, the $r_{\mathrm{rms}}$ stabilizes at seven major shells. The values are $r_{\mathrm{rms}} = 2.389$ fm, $r_{\mathrm{rms}} = 2.437$ fm and $r_{\mathrm{rms}} = 2.445$ fm for five, six and seven major oscillator shells, respectively. The experimental value is $r_{\mathrm{rms}} = 2.73 \pm 0.025$ fm.

Although we miss the experimental binding energy by 1 MeV per particle and the $r_{\mathrm{rms}}$ with some few per cent, our results show a saturation at around seven major oscillator shells. Furthermore, for nuclei like $^{16}$O, corrections from $T_3$ cluster to the ground state are small compared with the contributions at the CCSD level. This is an important message since it tells us that with the coupled-cluster methodology we can exhaust with good confidence various many-body contributions arising from a two-body interaction. The

Table 2
The excitation energies of $^4$He calculated using the oscillator basis states (in MeV).

| State | EOMCCSD | CR-CCSD(T) | CISD | Exact |
|---|---|---|---|---|
| J=1 | 11.791 | 12.044 | 17.515 | 11.465 |
| J=0 | 21.203 | 21.489 | 24.969 | 21.569 |
| J=2 | 22.435 | 22.650 | 24.966 | 22.697 |

remaining disagreement with experiment can then be retraced to missing contributions at the level of the initial hamiltonian (the two-body $G$-matrix), such as real three-body terms.

## 3. CONCLUSIONS AND FUTURE PLANS

Our experience thus far with the quantum chemistry inspired coupled cluster approximations to calculate the ground and excited states of the $^4$He and $^{16}$O nuclei indicates that this will be a promising method for nuclear physics. By comparing coupled cluster results with the exact results obtained by diagonalizing the Hamiltonian in the same model space, we demonstrated that relatively inexpensive coupled cluster approximations recover the bulk of the nucleon correlation effects in ground- and excited-state nuclei. These results are a strong motivation to further develop coupled cluster methods for the nuclear many-body problem, so that accurate *ab initio* calculations for small- and medium-size nuclei become as routine as in molecular electronic structure calculations.

Many-body methods like the coupled cluster approach offer possibilities for extending microscopic ab-initio calculations beyond nuclei like $^{40}$Ca. Furthermore, for weakly bound nuclei to be produced by future low-energy nuclear structure facilities it is almost imperative to increase the degrees of freedom under study in order to reproduce basic properties of these systems. Moving towards the driplines however the nuclei cease to be well bound, and coupling to continuum structures plays an important role, see for example the recent works on the *Gamow shell model* of Refs. [25,26]. We are presently working on deriving complex two-body effective interactions, see for example Ref. [27], for weakly bound systems, reflecting bound states, resonances and the non-resonant continuum. The coupled cluster methods can then be extended to studies of such systems through the inclusion of a complex hamiltonian. With the capability of the coupled cluster methods to handle increasing single-particle densities, demonstrated here for $^4$He and $^{16}$O, we believe that our methodology may offer a viable approach in studies of these nuclear systems.

We have based most of our analysis using two-body nucleon-nucleon interactions only. We feel this is important since techniques like the coupled cluster methods allow one to include a much larger class of many-body terms than done earlier. Eventual discrepancies with experiment such as the missing reproduction of e.g., the first excited $2^+$ state in a $1p0f$ calculation of $^{48}$Ca, can then be ascribed to eventual missing three-body forces, as indicated by the studies in Refs. [16,28,29] for light nuclei. The inclusion of real three-body interactions belongs to our future plans.

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