

COUPLED CLUSTER APPROACHES TO NUCLEI, GROUND STATES AND EXCITED STATES

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We present recent coupled-cluster studies of nuclei, with an emphasis on ground state and excited states properties of closed shell nuclei. Perspectives for future studies are delineated.

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 nuclear structure research facilities and the proposed Rare Isotope Accelerator 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-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.

The ab initio coupled-cluster theory is a particularly promising candidate for such endeavors due to its enormous success in quantum chemistry.

Here we describe applications of coupled cluster techniques to nuclear structure. The coupled-cluster methods are very promising, since they allow one to study ground- and excited-state properties of nuclei with dimensionalities beyond the capability of present shell-model approaches, with a much smaller numerical effort when compared to the more traditional shell-model methods aimed at similar accuracies. 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.

The coupled-cluster approach offers several advantages. It is fully microscopic and allows one to start with the free nucleon-nucleon interaction, or eventually three-body interaction models. It contains only linked diagrams, it is size extensive, and can be improved upon systematically, for example by the inclusion of three-body interactions and more complicated correlations. One can study both closed-shell systems and valence systems and it is possible to derive effective two and three-body interactions for open shell systems, with the inclusion of complex interactions, of great relevance for the study of weakly bound systems. Finally, it is amenable to parallel computing.

Here we present several coupled-cluster results from recent calculations with singles, doubles, and noniterative triples and their generalizations to excited states applied to the ^4He and ^{16}O nuclei. A comparison of coupled cluster results with the results of the exact diagonalization of the Hamiltonian in the same model space shows that the quantum chemistry inspired coupled cluster approximations provide an excellent description of ground and excited states of nuclei. The results presented here are a summary of recent works listed in Refs. ^{1,2}.

2. Coupled Cluster approach to Nuclei

Nuclear many-body theory often begins with a G -matrix interaction which is derived from an underlying bare nucleon-nucleon interaction. This G -matrix can in turn be used in perturbative many-body approaches in order to derive effective interactions for the nuclear shell model, see for example Refs. ^{3,4} for recent reviews. These approaches have shown to be rather successful in shell-model studies of several nuclear systems. However, to

derive effective interactions within the framework of many-body perturbation theory is 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. ⁵ 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.

An alternative to such resummation techniques is however offered by the so-called no-core approach. There one typically defines a two-body or three-body effective interaction within a large, but limited model space. This is parallel to our own approach below, where we limit the discussion to the no-core G -matrix so that all particles are active within our chosen model space. Using a given basis expansion of the many-body wave function we could then solve the nuclear problem by diagonalization as has been pursued by the no-core shell model collaboration ^{6,7,8,9}. In fact, the current and most advanced no-core techniques have approached ^{12}C , with nearly converged solutions ¹⁰.

It should be evident, however, that diagonalization procedures scale almost combinatorially with the number of particles in a given number of single-particle orbitals. Because of this scaling, diagonalization simply becomes untenable at some point. The efforts to expand diagonalization into p -shell nuclei with all nucleons active, an effort that spans over ten years, illustrates the problem. The computational complexity of the nucleus grows dramatically as the size of the nucleus increases. As a simple example consider oscillator single-particle states, and single-particle spaces consisting of 4 and 7 major oscillator shells, and compare the number of uncoupled many-body basis states there are for 4, 8, 12, and 16 particles. From table 1 we see an enormous growth of the standard shell-model diagonalization problem within the space. We calculated the number of $M = 0$ states for He and B within the model space consisting of 4 major shells and estimated the number of basis states for C and O. Also indicated are similar estimates for seven major oscillator shells. The important lesson to learn from these numbers is that the model-space expansion becomes astronomical quite quickly.

Yet, because of the advent of radioactive nuclear beam accelerators, such as the proposed Rare Isotope Accelerator (RIA) in the U.S., we face the daunting task of moving beyond p -shell nuclei in *ab initio* calculations.

Table 1. Dimensions of the shell-model problem in four major oscillator shells and 7 major oscillator shells with $M = 0$.

System	4 shells	7 shells
^4He	4E4	9E6
^8B	4E8	5E13
^{12}C	6E11	4E19
^{16}O	3E14	9E24

We should therefore investigate several ways of approaching the nuclear many-body problem in order to successfully make the move into the RIA era. Here we will discuss the coupled-cluster technique which can be used to pursue nuclear many-body calculations to heavier systems beyond the p -shell.

Coupled cluster theory originated in nuclear physics ^{11,12} around 1960. Early studies in the seventies ¹³ 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.* ¹⁴, for further theoretical development, and by Mihaila and Heisenberg ¹⁵, 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 15-20 years ^{16,17,18,19,20} 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, the method is size extensive which means that only linked diagrams appear in the computation of the energy (the expectation value of the Hamiltonian) and amplitude equations. As discussed in Ref. ¹⁶ 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 frag-

ments simultaneously. In chemistry, where the study of reactions is quite important, this is a crucial property not available in the interacting shell model (named configuration interaction in chemistry). Fourth, while the theory is not variational, 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.

We are in the process of applying quantum chemistry inspired coupled cluster methods^{16,17,18,19,20,21,22,23,24} to finite nuclei^{1,2}. We show one result from our current studies, namely the convergence of ¹⁶O as a function of the model space in which we perform the calculations.

The basic idea of coupled-cluster theory is that the correlated many-body wave function $|\Psi\rangle$ may be obtained by application of a correlation operator, T , such that

$$|\Psi\rangle = \exp(T) |\Phi\rangle, \quad (1)$$

where Φ is a reference Slater determinant chosen as a convenient starting point. For example, we use the filled 0s state as the reference determinant for ⁴He.

The cluster operator T is given by

$$T = T_1 + T_2 + \cdots T_A, \quad (2)$$

and represent various n -particle- n -hole (np - nh) excitation amplitudes such as

$$T_1 = \sum_{a \langle \varepsilon_f, i \rangle \varepsilon_f} t_a^i a_a^\dagger a_i, \quad (3)$$

$$T_2 = \frac{1}{4} \sum_{i,j \langle \varepsilon_f; ab \rangle \varepsilon_f} t_{ab}^{ij} a_a^\dagger a_b^\dagger a_j a_i, \quad (4)$$

and higher-order terms from 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

$$E_{\text{g.s.}} = \langle \Psi_0 | \exp(-T) H \exp(T) | \Psi_0 \rangle. \quad (5)$$

The Baker-Hausdorf relation may be used to rewrite the similarity transformation as an expansion in terms of nested commutators. The expansion terminates exactly at four nested commutators when the Hamiltonian contains, at most, two-body terms, and at six-nested commutators when

three-body potentials are present. This can also be seen diagrammatically, since $e^{-T}He^T$ is equivalent to the connected product of the Hamiltonian and e^T , which has to terminate at the quartic terms in T when interactions are pairwise (the Hamiltonian has at most four lines that can be connected with the T vertices) and at the T^6 terms when interactions are three-body (the Hamiltonian has at most six lines that can be connected with the T vertices). The equations for amplitudes are found by left projection of excited Slater determinants so that

$$\begin{aligned} 0 &= \langle \Phi_i^a | \exp(-T) H \exp(T) | \Phi \rangle, \\ 0 &= \langle \Phi_{ij}^{ab} | \exp(-T) H \exp(T) | \Phi \rangle. \end{aligned} \quad (6)$$

The commutators also generate nonlinear terms within these expressions. To derive these equations, we use the diagrammatic approach. In order to obtain the computationally efficient algorithms, which lead to the lowest operation count and memory requirements, we use the idea of recursively generated intermediates and diagram factorization¹⁷. 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.^{1,17}.

In our coupled-cluster study of Ref.¹, we performed calculations of the ^{16}O ground state for up to seven major oscillator shells as a function of $\hbar\omega$. Fig. 1 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 6.90 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.

We also considered chemistry inspired noniterative corrections to the CCSD energy due to three-body clusters T_3 (labelled triples in quantum chemistry). We performed this study in the model space consisting of four major oscillator shells, since we can perform exact shell-model calculations for nuclei such as ^4He . Table 2 shows the total ground-state energy val-

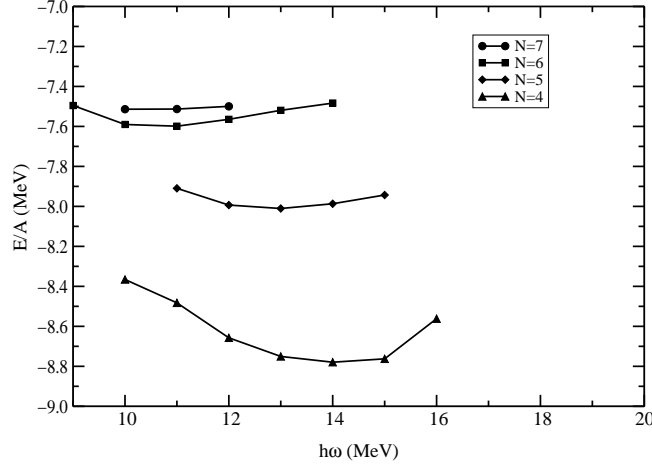


Figure 1. Dependence of the ground-state energy of ^{16}O on $\hbar\omega$ as a function of increasing model space.

ues obtained with the CCSD and one of the triples-correction approaches (labeled CR-CCSD(T) ^{19,20,25,26} 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. (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.

Table 2. The ground-state energy of ^{16}O calculated using various coupled cluster methods and oscillator basis states.

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

These results indicate that the bulk of the correlation energy within a nucleus can be obtained by solving the CCSD equations. This gives us confidence that we should pursue this method in open shell systems and to excited states. We have recently ² performed excited state calculations on ^4He using the EOMCCSD (equation of motion CCSD) method. For the excited states $|\Psi_K\rangle$ and energies $E_K^{(\text{CCSD})}$ ($K > 0$), we apply the EOM-CCSD (“equation of motion CCSD”) approximation ^{23,24} (equivalent to the response CCSD method ²⁷), in which

$$|\Psi_K\rangle = R_K^{(\text{CCSD})} \exp(T^{(\text{CCSD})}) |\Phi\rangle. \quad (7)$$

Here $R_K^{(\text{CCSD})} = R_0 + R_1 + R_2$ is a sum of the reference (R_0), one-body (R_1), and two-body (R_2) components obtained by diagonalizing $\bar{H}^{(\text{CCSD})}$ 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. These calculations may also be corrected in a non-iterative fashion using the completely renormalized theory for excited states ^{19,20,25,26,28}. 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 EOM-CCSD and CR-CCSD(T) are in excellent agreement with the exact results. We have recently also computed excited states in ^{16}O , with a particular em-

Table 3. The excitation energies of ^4He 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

phasis 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 very close 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 10 % 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. ²⁹.

Our experience thus far with the quantum chemistry inspired coupled cluster approximations to calculate the ground and excited states of the ^4He 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.

3. Perspectives and Future Plans

The study of exotic nuclei opens new challenges to nuclear physics. The challenges and the excitement arise because exotic nuclei will present new and radically different manifestations of nucleonic matter that occur near the bounds of nuclear existence, where the special features of weakly bound, quantal systems come into prominence. Furthermore, many of these nuclei are key to understanding matter production 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-mass nuclear systems. 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.

Many-body methods like the coupled cluster offer possibilities for extending microscopic *ab-initio* calculations to nuclei like ^{40}Ca . Especially the coupled-cluster methods are very promising, since they allow one to study

ground- and excited-state properties of nuclei with dimensionalities beyond the capability of present shell-model approaches. As demonstrated here and in Ref. ² we show for the first time how to calculate excited states for a nucleus using coupled cluster methods from quantum chemistry. For the 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. We are presently working on deriving complex effective interactions, see for example Ref. ³⁰, for weakly bound systems to be used in coupled cluster studies of these weakly bound nuclei.

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. ^{9,31,32,33,34,35} for light nuclei. The inclusion of real three-body interactions belongs to our future plans.

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References

1. D.J. Dean, and M. Hjorth-Jensen, Phys. Rev. **C69** (2004) 054320.
2. K. Kowalski, D.J. Dean, M. Hjorth-Jensen, T. Papenbrock, and P. Piecuch, Phys. Rev. Lett. **92** (2004) 132501.
3. M. Hjorth-Jensen, T.T.S. Kuo and E. Osnes, Phys. Rep. **261** (1995) 125.
4. D.J. Dean, T. Engeland, M. Hjorth-Jensen, M.P. Kartamyshev, and E. Osnes, Prog. Part. Nucl. Phys. **53** (2004) 419.
5. T. Helgaker, P. Jørgensen, and J. Olsen, *Molecular Electronic Structure Theory. Energy and Wave Functions*, (Wiley, Chichester, 2000).
6. P. Navrátil and B.R. Barrett, Phys. Rev. **C57** (1998) 562.
7. P. Navrátil, J.P. Vary, and B.R. Barrett Phys. Rev. Lett. **84** (2000) 5728.
8. P. Navrátil, J.P. Vary, and B.R. Barrett, Phys. Rev. **C62** (2000) 054311.
9. P. Navrátil and W.E. Ormand, Phys. Rev. Lett. **88** (2002) 152502.
10. A.C. Hayes, P. Navrátil, and J.P. Vary, Phys. Rev. Lett. **91** (2003) 012502.

11. F. Coester, Nucl. Phys. **7** (1958) 421.
12. F. Coester and H. Kümmel, Nucl. Phys. **17** (1960) 477.
13. H. Kümmel, K.H. Lührmann and J.G. Zabolitzky, Phys. Rep. **36** (1977) 1.
14. R.F. Bishop, E. Buendia, M.F. Flynn and R. Guardiola, J. Phys. G: Nucl. Part. Phys. **17** (1991) 857; *ibid.* **18** (1992) 1157; *ibid.* **19** (1993) 1663; R. Guardiola, P.I. Moliner, J. Navarro, R.F. Bishop, A. Puente and N.R. Walet, Nucl. Phys. **A609** (1996) 218; R.F. Bishop and R. Guardiola.
15. J.H. Heisenberg, and B. Mihaila, Phys. Rev. **C59** (1999) 1440
16. T.D. Crawford and H.F. Schaefer III, Rev. Comp. Chem. **14** (2000) 33..
17. S.A. Kucharski, R.J. Bartlett, Theor. Chim. Acta **80** (1991) 387; P. Piecuch, S.A. Kucharski, K. Kowalski, and M. Musiał, Comp. Phys. Comm, **149** (2002) 72, and references therein.
18. J. Paldus and X. Li, Adv. Chem. Phys. **110** (1999) 1.
19. P. Piecuch and K. Kowalski and I.S.O. Pimienta and M.J. McGuire, Int. Rev. Phys. Chem. **21** (2002) 527.
20. P. Piecuch and K. Kowalski and P.-D. Fan and I.S.O. Pimienta, eds. J. Maruani, R. Lefebvre and E. Brändas, *Topics in Theoretical Chemical Physics* vol. **12**, series Progress in Theoretical Chemistry and Physics, (Kluwer, Dordrecht, 2004) 119.
21. J. Čížek, J. Chem. Phys. **45** (1966) 4256.
22. J. Čížek, Adv. Chem. Phys. **14** (1969) 35.
23. J. F. Stanton and R. J. Bartlett, J. Chem. Phys. **98** (1993) 7029.
24. P. Piecuch and R. J. Bartlett, Adv. Quantum Chem. **34** (1999) 295.
25. K. Kowalski and P. Piecuch, J. Chem. Phys. **113** (2000) 18.
26. K. Kowalski and P. Piecuch, J. Chem. Phys. **120** (2004) 1715.
27. H. Monkhorst, Int. J. Quantum Chem. Symp. **11** (1977) 421.
28. K. Kowalski and P. Piecuch, J. Chem. Phys. **115** (2001) 2966.
29. M. Wloch, D.J. Dean, J.P. Gour, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, and P. Piecuch, in preparation for Phys. Rev. Lett.
30. G. Hagen, J.S. Vaagen, and M. Hjorth-Jensen, J. Phys. A:Math. Gen. **37** (2004) 8991.
31. S.C. Pieper, V.R. Pandharipande, R.B. Wiringa, and J. Carlson, Phys. Rev. **C64** (2001) 014001
32. S.C. Pieper, K. Varga, and R.B. Wiringa, Phys. Rev. **C66** (2002) 0044310
33. R.B. Wiringa and S.C. Pieper, Phys. Rev. Lett. **89** (2002) 182501
34. A. Akmal, V.R. Pandharipande and D.G. Ravenhall, Phys. Rev. **C58** (1998) 1804.
35. P. Navrátil and W.E. Ormand, Phys. Rev. **C68** (2003) 034305.