# COUPLED-CLUSTER THEORY FOR NUCLEI

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## 1. INTRODUCTION

The quantum many body problem spans numerous scientific disciplines ranging from condensed matter to quantum dots, to high-temperature superconductors, and to nuclei. In these Proceedings, we discuss the development of coupled-cluster techniques and their application to nuclei. We concentrate specifically on calculations pertaining to the ground- and excited-state properties of $^{16}$O.

The coupled-cluster method originated in nuclear physics over forty years ago when Coester and Kummel proposed an exponential ansatz to describe correlations within a nucleus [1,2]. This ansatz has been well justified for many-body problems using a formalism in which the cluster functions are constructed by cluster operators acting on a reference determinant [3]. Early applications to finite nuclei were described in Ref. [4]. From that time to this, a systematic development and implementation of this interesting many-body theory in nuclear physics applications has been only sporadic. The view from computational quantum chemistry is quite different. In fact, beginning with its introduction into quantum chemistry by Čížek [5], coupled-cluster methods have enjoyed tremendous success [6,7,8,9,10] over a broad class of problems related to chemical and molecular structure and chemical reactions.

In this work, we apply coupled-cluster methods to nuclei with 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 one-hundred correlated electrons, we anticipate that quantum-chemistry inspired coupled-cluster approaches will enable accurate studies of ground and excited states of nuclei with many-body dimensions beyond the capability of present shell-model approaches (also known as Hamiltonian diagonalization or configuration-interaction 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 nuclei whose dimensionality is beyond reach for present shell-model studies. Today's typical limits on shell-model diagonalization are on the order of $10^9$ many-body basis states [11].

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 nucleus, one exactly produces the fully correlated many-body wave function of the system. We show below how the improvements affect the ground- and excited-state energies in $^{16}$O. The only input that the method requires is the nucleon-nucleon interaction. The method may also be extended to incorporate three-nucleon interactions. 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, for example in 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 is 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 and 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.

In these Proceedings, we present our approach to the nuclear many-body problem using coupled-cluster theory. In Section 2, we briefly describe the formalism we employ. In Section 3, we present results in $^{16}$O, and conclude with an outlook in Section 4.

## 2. FORMALISM

We use two variants of effective field theory-inspired Hamiltonians which are the Idaho-A [12] and N3LO [13]. The Idaho-A potential was derived with up to chiral-order three diagrams, while N3LO includes chiral-order four diagrams, charge

symmetry-breaking, and charge independence-breaking terms. We also include point Coulomb in the N3LO calculations presented below. While earlier coupled-cluster calculations [14] used bare interactions, we renormalize the bare Hamiltonian using a no-core G-matrix approach [15,16] which obtains a starting-energy dependence $\tilde{\omega}$ in the two-body matrix elements $G(\tilde{\omega})$.

A common practice in nuclear many-body theory is to reduce the infinitely many degrees of freedom of the Hilbert space to those represented by a physically motivated subspace, the model space. In such truncations of the Hilbert space, the notions of a projection operator $P$ onto the model space and its complement $Q$ are introduced. The projection operators defining the model and excluded spaces are

$$P = \sum_{i=1}^{D} |\Phi_i\rangle \langle\Phi_i| , \tag{1}$$

and

$$Q = \sum_{i=D+1}^{\infty} |\Phi_i\rangle \langle\Phi_i| , \tag{2}$$

with $D$ being the dimension of the model space, and $PQ = 0$, $P^2 = P$, $Q^2 = Q$, and $P + Q = I$. The two-body wave functions $|\Phi_i\rangle$ are normally eigenfunctions of an unperturbed Hamiltonian $H_0$. In this work we let only the kinetic energy enter the definition of $H_0$, i.e., $H_0 = t$. Since we will employ a harmonic oscillator basis, this means that we need to compute the expectation value of $H_0$ as well. The unperturbed wave functions are not eigenfunctions of $t$. The full Hamiltonian is then $H = t + V_{NN}$, with $V_{NN}$ the nucleon-nucleon interaction. The eigenfunctions of the full two-body Hamiltonian are denoted by $|\Psi_\alpha\rangle$ and $E_\alpha$,

$$H |\Psi_\alpha\rangle = E_\alpha |\Psi_\alpha\rangle . \tag{3}$$

Rather than solving the full Schrödinger equation above, we define an effective Hamiltonian acting within the model space such that

$$PH_{\text{eff}}P |\Psi_\alpha\rangle = E_\alpha P |\Psi_\alpha\rangle = E_\alpha |\Phi_\alpha\rangle \tag{4}$$

where $|\Phi_\alpha\rangle = P |\Psi_\alpha\rangle$ is the projection of the full wave function onto the model space, and is called the model space wave function. Here $H_{\text{eff}}$ is an effective Hamiltonian acting solely within the chosen model space given by $H_{\text{eff}} = PtP + V_{\text{eff}}$, with the interaction

$$V_{\text{eff}} = \sum_{i=1}^{\infty} V_{\text{eff}}^{(i)}, \tag{5}$$

where $V_{\text{eff}}^{(1)}$, $V_{\text{eff}}^{(2)}$, $V_{\text{eff}}^{(3)}$,... are effective one-body, two-body, three-body interactions, etc. For finite $A$-body systems, the sum terminates at $i = A$. As stated above, in this work we will limit the attention to two-body interactions. The next step could be to employ perturbative many-body techniques or the coupled-cluster method. In perturbation theory, the effective interaction $H_{\text{eff}}$ can be written out order by order in the interaction $V_{NN}$ as

$$PH_{\text{eff}}P = PtP + PV_{NN}P + PV_{NN}\frac{Q}{e}V_{NN}P + PV_{NN}\frac{Q}{e}V_{NN}\frac{Q}{e}V_{NN}P + \ldots . \tag{6}$$

In this expansion, $e = \omega - t$, where $\omega$ is the so-called starting energy, defined as the unperturbed energy of the interacting particles. However, the nucleon-nucleon interactions all possess a hard core that makes them unsuitable for perturbative many-body approaches. The standard procedure is therefore to renormalize the short-range part of the interaction by introducing the so-called reaction matrix $G$

$$G = V_{NN} + V_{NN} \frac{\tilde{Q}}{\omega - \tilde{Q} t \tilde{Q}} G. \tag{7}$$

The operator $\tilde{Q}$ is normally different from the projection operator defined in Eq. (2), since the $G$-matrix by construction allows only specific two-body states to be defined by $\tilde{Q}$. Typically, the $G$-matrix is the sum over all ladder types of diagrams with intermediate particle-particle states only. This sum is meant to renormalize the repulsive short-range part of the interaction. The physical interpretation is that the particles must interact with each other an infinite number of times in order to produce a finite interaction. This interaction can in turn serve as an effective interaction acting in a reduced space.

The unperturbed Hamiltonian $H_0$ is given by the kinetic energy only. However, in order to define a suitable starting point for an effective interaction to be used in the coupled-cluster calculations, we use complete oscillator shells as our basis states and define our particles and holes in terms of the naive filling of oscillator states for a given nucleus. For example, for $^4$He, the reference Slater determinant is the filled $0s$ shell (for both protons and neutrons), and the filled $0s$-$0p$ shells for $^{16}$O. We compute the single-hole energies $\varepsilon_i$ through

$$\varepsilon_i = \langle i | \frac{p^2}{2m} | i \rangle + \sum_{j \leq F} \langle ij | \, G(\omega = \varepsilon_i + \varepsilon_j) \, | ij \rangle \,, \tag{8}$$

where $F$ stands for the Fermi energy. Here we introduce the notation that $i, j, k, l$ refer to single-hole states, $a, b, c, d$ refer to single particle states, and $p, q, r, s$ refer to all single-particle states. We do not perform a self-consistent Brueckner-Hartree-Fock calculation however, as done by, e.g., Gad and Müther [17]. The matrix elements are all antisymmetrized. Furthermore, for single-particle states above the Fermi energy we leave the single-particle energies unchanged. This procedure, which follows the Bethe-Brandow-Petschek theorem [18], introduces an artificial gap at the Fermi surface. Note also that the single-particle wave functions are not changed in Eq. (8). The main purpose of the above procedure is to yield a prescription for obtaining a starting energy independent effective interaction for the coupled-cluster calculations. Using the single-particle energies from Eq. (8), we define, following Ref. [17], an effective interaction for our coupled-cluster model spaces by

$$\langle ij | \, \mathcal{V}_{\text{eff}} \, | kl \rangle = \frac{1}{2} \left[ \langle ij | \, G(\omega = \varepsilon_i + \varepsilon_j) \, | kl \rangle \, + \, \langle ij | \, G(\omega = \varepsilon_k + \varepsilon_l) \, | kl \rangle \right], \tag{9}$$

for two-body states with holes only and

$$\langle ip | \, \mathcal{V}_{\text{eff}} \, | kq \rangle = \frac{1}{2} \left[ \langle ip | \, G(\omega = \varepsilon_i + \varepsilon_p) \, | kq \rangle \, + \, \langle ip | \, G(\omega = \varepsilon_k + \varepsilon_q) \, | kq \rangle \right], \tag{10}$$

for two-body states with one particle and one hole. For two-body states with two single-particle states $pq$, we use a fixed starting energy, typically in the range $\omega \in [-80, -5]$ MeV. This introduces a starting energy dependence in our results. The reason for fixing the starting energies for two-particle states is due to the fact that we use kinetic energies only above the Fermi surface and our $G$-matrices are computed at negative starting energies only.

Our starting point for coupled-cluster calculations is then $H' = t + G(\tilde{\omega})$. We correct for center-of-mass contaminations using $H = H' + \beta_{\rm c.m.} H_{\rm c.m.}$, given at $\beta_{\rm c.m.}$ where $\langle H_{\rm c.m.} \rangle = 0.0$ MeV.

The correlated many-body wave function of the coupled-cluster method is given by $\mid \Psi\rangle = \exp(T) \mid \Phi\rangle$ where $T = T_1 + T_2 + \cdots$ is the cluster operator, and the one-particle-one-hole cluster operator is $T_1 = \sum_{a,i} t_i^a a_a^\dagger a_i$, while the two-particle-two-hole cluster is $T_2 = \frac{1}{4} \sum_{ab,ij} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$. Similar definitions exist for higher-order clusters. The CCSD (coupled clusters in singles and doubles) keeps only the $T_1$ and $T_2$ terms in the correlation operator. Equations for the cluster amplitudes can be derived by applying diagrammatic or algebraic techniques of many-body theory to the expressions $\langle \Phi_i^a \mid \bar{H} \mid \Phi \rangle = 0$ and $\langle \Phi_{ij}^{ab} \mid \bar{H} \mid \Phi \rangle = 0$, where $\bar{H} = \exp(-T) H \exp(T)$ and $T^{(\rm CCSD)} = T_1 + T_2$. These expressions yield a set of energy independent, coupled, non-linear algebraic equations for the cluster amplitudes $t_i^a$ and $t_{ij}^{ab}$ that may be solved iteratively.

For the excited states $|\Psi_K\rangle$ and energies $E_K^{(\rm CCSD)}$ ($K > 0$), we apply the EOM-CCSD ("equation of motion CCSD") approximation [19,20] (equivalent to the linear response and time-dependent CCSD methods [21]; cf. Refs. [22,23,20,24]), in which $|\Psi_K\rangle = R_K^{(\rm CCSD)} \exp(T^{(\rm CCSD)}) |\Phi\rangle$. Here $R_K^{(\rm CCSD)} = R_0 + R_1 + R_2$ is a sum of the reference ($R_0$), one-body ($R_1$), and two-body ($R_2$) components obtained by diagonalizing $\bar{H}$ 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.

Noniterative triples corrections to the energy, arising from the inclusion of three-body clusters, $T_3$ and three-body ($R_3$) components to the linear excitation operator $R_K$, can be calculated by using completely renormalized coupled-cluster theory [25,26,27,28] (shown here for the ground-state). The completely renormalized coupled-cluster theory relies on the fact that if the exact wave function, $\mid \Psi_0\rangle$ is known then the difference $\delta$ between the exact energy $E_0$ and the CCSD energy $E_0^{(\rm CCSD)}$ equals the coupled-cluster generating functional evaluated at $\mid \Psi_0\rangle$:

$$\Lambda_{\rm CC}[\Psi_0] = \frac{\sum_{n=1}^{N} \langle \Psi_0 \mid Q_n \left( H - E_0^{(\rm CCSD)} \right) \exp(T^{(\rm CCSD)}) \mid \Phi \rangle}{\langle \Psi_0 \mid \exp(T^{(\rm CCSD)}) \mid \Phi \rangle} \,, \tag{12}$$

where $Q_n$ is a projector onto $n$-particle-$n$-hole states. If we first solve the CCSD equations, then the leading term in the correction $\delta$ to the CCSD energy, due to three-particle-three-hole excitations that can be extracted from Eq. (12), becomes $\delta = \frac{1}{36\Delta} \sum_{abc,ijk} \langle \tilde{\Psi} \mid \Phi_{ijk}^{abc} \rangle M_{abc}^{ijk}$, where the moments of the coupled-cluster equation are given by $M_{abc}^{ijk} = \langle \Phi_{ijk}^{abc} \mid \bar{H} \mid \Phi \rangle$, $\Delta = \langle \tilde{\Psi} \mid \exp(T^{(\rm CCSD)}) \mid \Phi \rangle$, and $\mid \tilde{\Psi} \rangle = P \exp(T^{(\rm CCSD)} + \tilde{T}_3)$, where $P$ projects onto the space spanned by the reference determinant $\mid \Phi\rangle$ and all one-particle-one-hole, two-particle-two-hole, and three-particle-

three-hole excited determinants. Also, $\tilde{T}_3 = \frac{1}{36}\sum_{ijk,abc}\left(\mathcal{M}^{ijk}_{abc}/D^{abc}_{ijk}\right) a^\dagger_a a^\dagger_b a^\dagger_c a_j a_k a_i$. The quantities are easily calculable. We apply the completely renormalized approach to calculations of both ground and excited states in our nuclear systems [29,30]. on previous work, the definition of $D^{abc}_{ijk}$ is given by variant "c" of the CR-CCSD(T) and CR-EOMCCSD(T) approaches [29].

## 3. RESULTS and DISCUSSION

We first discuss ground-state results for $^{16}$O. Shown in Fig. (1) is a graphical representation of a compendium of results from our calculations. In the top panel of Fig. (1) we show the convergence of the ground-state energy calculated with CCSD and with CR-CCSD(T). We were able to perform the CCSD calculations with up to 8 major oscillator shells. The symbols in the figure represent our calculations, while the lines represent a fit function of the form $E(N) = E_\infty + a\exp(-b\cdot N)$, where $E_\infty$ is the extrapolated energy and $a$ and $b$ are coefficients for the fit. We show in the middle panel of Fig. (1) our EOMCCSD and CR-EOMCCSD(T) calculations for the first excited $3^-$ state, while the lower panel indicates the position of the lowest $0^+$ state in our calculations. We comment on these three results in the following paragraphs.

We indicated in previous work [29] that the triples corrections from CR-CCSD(T) calculations to the ground-state CCSD energies are small in a basis including four major oscillator shells. We extended these calculations to 8 major oscillator shells for CCSD ground-state calculations and 7 major oscillator shells for CR-CCSD(T) calculations, as shown in Fig. (1). We find that the extrapolated CCSD energy is $E_0^{(\mathrm{CCSD})}$ =-119.42 MeV for Idaho-A. Our results indicate that triples corrections to the ground-state energy in $^{16}$O are less than 1% of the total energy. For the $N = 7$ calculation, the difference between the CCSD and CR-CCSD(T) result is 0.6 MeV, while the extrapolated values differ by only 1.05 MeV; our extrapolated CR-CCSD(T) energy is then -120.5 MeV. Coulomb would add to the binding approximately 11.2 MeV, so that our estimated Idaho-A ground state energy is -109.3 MeV (compared to an experimental value of -128 MeV). Our nearly converged N3LO CCSD energy (at $N = 8$ oscillator shells) is -111.2 MeV. Thus the two-body interactions underbind $^{16}$O by approximately 1 MeV per particle, leaving room for extra binding to be generated by the a three-body interaction. For the Idaho-A and N3LO interactions and the closed-shell $^{16}$O nucleus we conclude that connected-triples amplitudes are indeed quite small and contribute little to the ground-state energy.

The first excited $3^-$ state in $^{16}$O is thought to be principally a one-particle-one-hole state [32]. The CCSD and CR-CCSD(T) methods for excited states should well describe such a state as they account for all one-particle-one-hole excitations within the space. The largest $R_1$ amplitudes indicate that the dominant excitations are from the $0p_{1/2}$ orbital to the $0d_{5/2}$ orbital. $R_2$ and $R_3$ amplitudes are much smaller than the $R_1$ amplitudes, and the completely renormalized calculation hardly changes the total energy of the state. Our extrapolated results indicate that the $3^-$ state lies at -108.2 MeV, and -108.4 MeV in EOMCCSD and CR-EOMCCSD(T), respectively. The completely renormalized results yield an excitation energy of 12.3 MeV for this state which experimentally lies at 6.12 MeV of excitation. N3LO yields similar re-

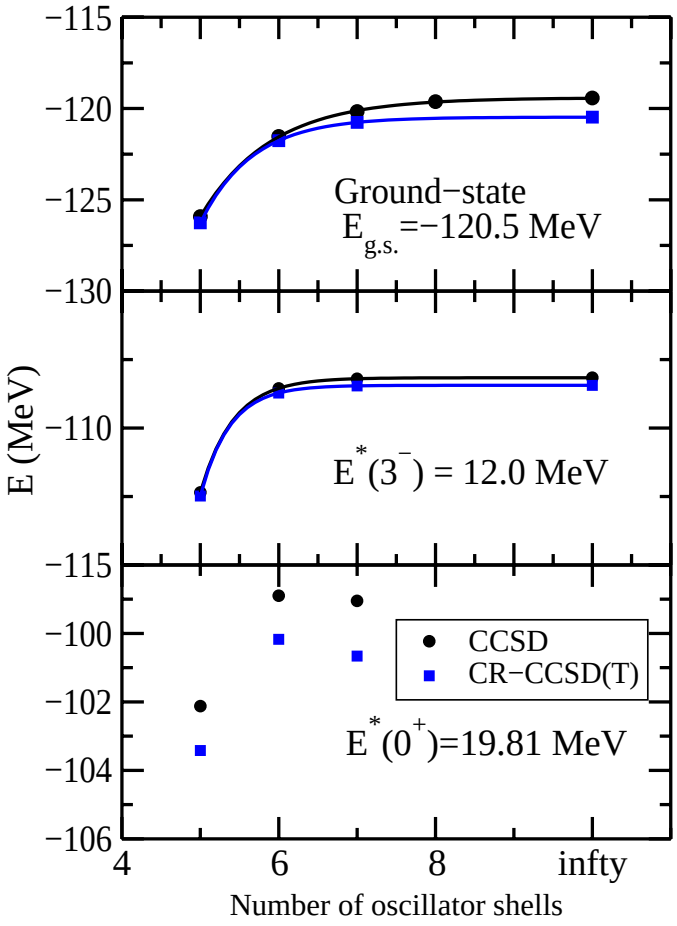


**Figure 1.** Top panel: the ground-state energy; middle panel: energy of the first excited $3^-$; bottom panel: first excited $0^+$. All quantities are given as a function of oscillator space size. Triples corrections are also applied. Extrapolations to the infinite space size are also shown.

sults. Based on the $1p$-$1h$ structure of the state, we can conclude that Idaho-A and N3LO do not yield an excitation energy for the $3^-$ which is commensurate with experiment which again points to the likely need to include three-body forces in nuclear calculations.

The first excited $0^+$ state is believed to be a $4p$-$4h$ state and should not be described at the EOMCCSD or CR-EOMCCSD(T) level. In fact we see significant differences between the standard EOM and completely renormalized calculations, as shown in the lower panel of Fig. (1). In this case, the Hamiltonian cannot be blamed for the inability to reproduce the correct excitation energy since one would need to include $4p$-$4h$ excitations to more accurately calculate this lowest $0^+$ excited state.

## 4. FUTURE DIRECTIONS

$^{16}$O represents an interesting nucleus and these calculations are among the first to probe, from an *ab initio* point of view, the structure of both its ground- and excited states. This research will further develop in several directions. The $G$-matrix calculations for the effective interaction will eventually be replaced by a similarity transform approach [32]. This approach can be used to eliminate any starting-energy dependence in the $G$-matrix. We will also investigate the use of $G$-matrices that are better suited for studies of weakly bound nuclei where an appropriate description of the single-particle states within the continuum is necessary [33]. We will also extend our CCSD and CR-CCSD(T) calculations and the excited state calculations to open-shell nuclei and properties other than energy.

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