

Coupled-cluster calculations for ground and excited states of closed- and open-shell nuclei using methods of quantum chemistry

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Abstract

We discuss large-scale *ab initio* calculations of ground and excited states of ^{16}O and preliminary calculations for ^{15}O and ^{17}O using coupled-cluster methods and algorithms developed in quantum chemistry. By using realistic two-body interactions and the renormalized form of the Hamiltonian obtained with a no-core G-matrix approach, we are able to obtain the virtually converged results for ^{16}O and promising results for ^{15}O and ^{17}O at the level of two-body interactions. The calculated properties other than binding and excitation energies include charge radius and charge form factor. The relatively low costs of coupled-cluster calculations, which are characterized by the low-order polynomial scaling with the system size, enable us to probe large model spaces with up to seven or eight major oscillator shells, for which nontruncated shell-model calculations for nuclei with $A = 15$ –17 active particles are presently not possible.

1. Introduction

One of the most important problems in nuclear physics is to understand how various properties, such as masses and excitation spectra, arise from the underlying nucleon–nucleon interactions. While significant progress has been made in the development of Green's function

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Monte Carlo [1] and no-core shell model [2] techniques, which have produced converged results for nuclei with up to $A = 12$ nucleons, the applicability of these methods is limited to light nuclei. Given that present nuclear structure research facilities and the proposed Rare Isotope Accelerator will continue to provide more and more information about the properties of medium-mass and heavier nuclei, it becomes critical to examine alternative approaches to the nuclear many-body problem that could eventually be applied to medium-size systems in the mass 50 region. Coupled-cluster methods based on the exponential wavefunction ansatz [3, 4], which we discuss in this paper, are promising candidates for reliable *ab initio* calculations for medium-size nuclei due to their ability to provide precise description of many-particle correlation effects at a relatively low computer cost when compared to shell-model or configuration interaction techniques aimed at similar accuracies, as has been demonstrated over and over again in numerous chemistry applications (see, e.g., [5–8] for reviews).

Historically, coupled-cluster theory originated in nuclear physics [3], but its applications to the nuclear many-body problem have been relatively rare (see, e.g., [9]). This should be contrasted with the situation in chemistry. After the introduction of the coupled-cluster wavefunction ansatz and diagrammatic methods of many-body theory into quantum chemistry by Čížek [4] and after the early exploration of coupled-cluster techniques in molecular applications by Čížek, Paldus and their collaborators, which was followed by the development of general-purpose coupled-cluster computer codes, primarily by Bartlett's, Pople's and Schaefer's groups (see, e.g., [6] for historical remarks), coupled-cluster methods have enjoyed tremendous success over a broad range of problems related to molecular structure, properties and reactivity. Many kinds of coupled-cluster methods have been developed for closed-shell, open-shell, nondegenerate, and quasi-degenerate ground and excited states of many-electron systems [5–8]. In consequence, coupled-cluster methods of the type of the single-reference approximations discussed in this paper are nowadays routinely applied to many-electron systems containing dozens of light atoms, several transition metal atoms, hundreds of electrons and thousands of basis functions (see, e.g., [10, 11]). In fact, many coupled-cluster methods are available in the popular quantum chemistry software packages, enabling highly accurate *ab initio* calculations of useful molecular properties by nonexperts. Significant progress has also been made to convert even more powerful multi-reference coupled-cluster techniques into practical computational algorithms that can be applied to a growing number of problems involving many-electron systems (cf, e.g., [6, 12, 13] for selected recent examples). We believe that the field of nuclear physics may significantly benefit from vast experience in the development of reliable and computationally efficient coupled-cluster methods by quantum chemists.

Recent coupled-cluster calculations for light nuclei, using modern nucleon–nucleon interactions and approximations similar to those used by quantum chemists, have demonstrated that one may be able to overcome the computational bottlenecks posed by the prohibitive costs of the shell-model and Monte Carlo calculations. In particular, using bare interactions, Mihaila and Heisenberg performed coupled-cluster calculations for the binding energy and the electron scattering form factor of ^{16}O [14–17]. In the previous work [18], we took an alternative route and used a few quantum chemistry inspired coupled-cluster techniques, and the renormalized form of the Hamiltonian, to calculate ground and excited states of ^4He and ground-state energies of ^{16}O in a small model space consisting of four major oscillator shells, demonstrating promising results when compared with the results of the exact shell-model diagonalization.

This paper highlights the results of our large-scale calculations of ground- and excited-state energies and selected properties of ^{16}O [19] obtained with the efficient coupled-cluster codes for nuclear structure that we developed in recent months using the elegant diagram-

factorization techniques exploited by quantum chemists [20–22]. We also report the results of preliminary coupled-cluster calculations for two open-shell nuclei, ^{15}O and ^{17}O . There are several differences between our approach to nuclear coupled-cluster calculations and the approach pursued earlier by Mihaila and Heisenberg [14–17]. First of all, Mihaila and Heisenberg use bare interactions, making the convergence with the number of single-particle basis states very slow, whereas we use the renormalized form of the Hamiltonian exploiting a no-core G -matrix theory [23], which leads to a rapid convergence of binding and excitation energies and other nuclear properties with the number of major oscillator shells in a basis. Second, we are able to calculate ground and excited states of open-shell nuclei. Finally, as already mentioned above, our coupled-cluster computer codes have been developed using diagram-factorization techniques, which minimize the operation count, rather than the commutator expansions used by Mihaila and Heisenberg and the Bochum school.

The ground- and excited-state energies of ^{16}O reported in this work were calculated in basis sets consisting of up to eight major oscillator shells (480 single-particle states), whereas the properties other than energy, such as charge radius and charge form factor, were obtained in basis sets consisting of up to seven major oscillator shells (336 single-particle states). The preliminary results for ^{15}O and ^{17}O were performed with five and six major oscillator shells. All of this represents significant progress compared to our earlier calculations [18], in which we had to limit ourselves to 80 single-particle states, closed-shell nuclei and energy calculations only.

2. Brief description of theory and computational details

In general, all coupled-cluster methods are classified as either the single-reference approaches or multi-reference methods (see, e.g., [6, 12, 13]). In this paper, we focus on the single-reference coupled-cluster methods, in which the correlated wavefunctions of the A -body system are constructed via particle–hole (p–h) excitations from a single determinant.

2.1. Effective Hamiltonian

In calculations for ^{16}O , we used two potentials derived from the effective field theory [24, 25], namely, Idaho-A [26] and N3LO [27]. The Idaho-A potential is derived with up to chiral-order three diagrams, while N3LO includes chiral-order four diagrams and charge-symmetry and charge-independence breaking terms. We also include the Coulomb interaction in N3LO, which is not included in Idaho-A. In calculations for ^{15}O and ^{17}O , we used the N3LO potential only (to distinguish between $^{15}\text{O}/^{17}\text{O}$ and $^{15}\text{N}/^{17}\text{F}$). In order to remove the hard-core part of the interaction that would require calculations in extremely large model spaces to reach converged results [14–17] and enable realistic calculations in manageable model spaces, we renormalize the Hamiltonian through a no-core G -matrix procedure [23]. The no-core G -matrix approach introduces a starting-energy ($\tilde{\omega}$) dependence in the effective two-body matrix elements $G(\tilde{\omega})$ defining the renormalized two-body interactions, but much of the $\tilde{\omega}$ dependence can be eliminated through the use of the Bethe–Brandow–Petschek theorem [28] (see [23] for details). After renormalizing bare interactions, our Hamiltonian is given by the formula $H' = t + G(\tilde{\omega})$, where t is the kinetic energy. We correct the renormalized Hamiltonian H' for centre-of-mass (c.o.m.) contaminations using the expression $H = H' + \beta_{\text{c.m.}} H_{\text{c.m.}}$, where $\beta_{\text{c.m.}}$ is chosen such that the expectation value of the c.o.m. Hamiltonian $H_{\text{c.m.}}$ is 0.0 MeV. One of the advantages of this procedure is the ease of separation of intrinsic and c.o.m. contaminated states by analyzing the dependence of coupled-cluster energies on $\beta_{\text{c.m.}}$.

Table 1. The $\beta_{\text{c.m.}}$ dependence of the excitation energies for the lowest-energy 3^- state of ^{16}O obtained with the EOMCCSD approach, Idaho-A and a basis set of five major oscillator shells (excitation energies and $\beta_{\text{c.m.}}$ values in MeV).

$\beta_{\text{c.m.}} = 0.5$	$\beta_{\text{c.m.}} = 1.0$	$\beta_{\text{c.m.}} = 1.5^a$
13.413	13.497	13.574

^a The optimum value of $\beta_{\text{c.m.}}$ giving the expectation value of $H_{\text{c.m.}}$ of 0.0 MeV.

As shown in table 1, the physical states obtained in coupled-cluster calculations are virtually independent of $\beta_{\text{c.m.}}$.

2.2. Coupled-cluster calculations

Once the one- and two-body matrix elements of the c.o.m.-corrected renormalized Hamiltonian H are determined and properly sorted out, we solve the nuclear many-body problem using coupled-cluster theory. Our calculations always begin with the basic CCSD ('coupled-cluster singles and doubles') calculations, which provide information about the correlated ground state $|\Psi_0\rangle$ of a closed-shell system (e.g., ^{16}O). The CCSD method [29] is obtained by truncating the many-body expansion for the cluster operator T in the exponential wavefunction ansatz defining the ground-state coupled-cluster theory, $|\Psi_0\rangle = \exp(T)|\Phi\rangle$, where $|\Phi\rangle$ is the reference determinant, at the 2p–2h component T_2 . Thus, the truncated cluster operator T used in the CCSD calculations is $T = T_1 + T_2$, where $T_1 = t_a^i a^a a_i$ and $T_2 = \frac{1}{4} t_{ab}^{ij} a^a a^b a_j a_i$ are the singly and doubly excited clusters, i, j, \dots (a, b, \dots) are the single-particle states occupied (unoccupied) in the reference determinant $|\Phi\rangle$, a^p (a_p) are the creation (annihilation) operators associated with the orthonormal single-particle states $|p\rangle$ and the Einstein summation convention over repeated upper and lower indices is employed. The singly and doubly excited cluster amplitudes t_a^i and t_{ab}^{ij} that define the T_1 and T_2 operators, respectively, are obtained by solving the nonlinear system of coupled, energy-independent, algebraic equations, $\langle \Phi_i^a | \bar{H} | \Phi \rangle = 0$, $\langle \Phi_{ij}^{ab} | \bar{H} | \Phi \rangle = 0$, where $\bar{H} = \exp(-T) H \exp(T)$, and $|\Phi_i^a\rangle = a^a a_i |\Phi\rangle$ and $|\Phi_{ij}^{ab}\rangle = a^a a^b a_j a_i |\Phi\rangle$ are the singly and doubly excited determinants, respectively, relative to $|\Phi\rangle$. The computationally convenient form of these and other equations used in coupled-cluster calculations, in terms of matrix elements of the Hamiltonian H and cluster amplitudes t_a^i and t_{ab}^{ij} , can be best derived by applying diagram-factorization methods [20–22]. Once t_a^i and t_{ab}^{ij} are determined, the ground-state CCSD energy is calculated as $E_0 = \langle \Phi | \bar{H} | \Phi \rangle$.

For the excited states $|\Psi_\mu\rangle$, we use the equation of motion (EOM) CCSD approach [30], in which $|\Psi_\mu\rangle = R^{(\mu)} \exp(T) |\Phi\rangle$ (see, also, [31] and references therein). Here, $T = T_1 + T_2$ and $R^{(\mu)} = R_0 + R_1 + R_2$ is a linear excitation operator, where $R_0 = r_0 \mathbf{1}$, $R_1 = r_a^i a^a a_i$ and $R_2 = \frac{1}{4} r_{ab}^{ij} a^a a^b a_j a_i$ are the reference, one-body and two-body components of $R^{(\mu)}$. The excitation amplitudes r_a^i and r_{ab}^{ij} and the corresponding excitation energies ($E_\mu - E_0$) are determined by diagonalizing the similarity transformed Hamiltonian \bar{H} in the space spanned by singly and doubly excited determinants $|\Phi_i^a\rangle$ and $|\Phi_{ij}^{ab}\rangle$. The coefficient r_0 at the reference determinant $|\Phi\rangle$ in the EOMCCSD wavefunction $|\Psi_\mu\rangle$ is calculated *a posteriori* using the equation $r_0 = \langle \Phi | [\bar{H}(R_1 + R_2)]_C | \Phi \rangle / (E_\mu - E_0)$, where the subscript C represents the connected part of the corresponding operator product. The similarity transformed Hamiltonian \bar{H} is not Hermitian, so that in addition to the right eigenstates $R^{(\mu)} |\Phi\rangle$, which determine the 'ket' coupled-cluster wavefunctions $|\Psi_\mu\rangle$, we can also calculate the left eigenstates of \bar{H} , $\langle \Phi | L^{(\mu)}$, which define the 'bra' wavefunctions $\langle \Psi_\mu | = \langle \Phi | L^{(\mu)} \exp(-T)$ [30, 31]. Here, $L^{(\mu)}$

is a hole-particle deexcitation operator, so that $L_1 = l_i^a a^i a_a$ and $L_2 = \frac{1}{4} l_{ij}^{ab} a^i a^j a_b a_a$. The right and left eigenstates of \bar{H} form a biorthonormal set, $\langle \Phi | L^{(\mu)} R^{(v)} | \Phi \rangle = \delta_{\mu\nu}$. The left eigenstates $\langle \Phi | L^{(\mu)}$ are needed if we want to calculate properties other than energy. Indeed, the expectation values and transition matrix elements involving coupled-cluster states $\langle \tilde{\Psi}_\mu |$ and $|\Psi_\nu\rangle$ are calculated as $\langle \tilde{\Psi}_\mu | \theta | \Psi_\nu \rangle = \langle \Phi | L^{(\mu)} \bar{\theta} R^{(v)} | \Phi \rangle$, where $\bar{\theta} = \exp(-T) \theta \exp(T)$ is a similarity-transformed property operator θ . In particular, when $\theta = a^p a_q$ and $\mu = \nu$, we can determine the CCSD or EOMCCSD one-body reduced density matrices in quantum states $|\Psi_\mu\rangle$ and the corresponding one-body properties (in the CCSD ground-state case, where $T = T_1 + T_2$, we have $R^{(0)} = \mathbf{1}$ and $L^{(0)} = 1 + \Lambda_1 + \Lambda_2$, where Λ_1 and Λ_2 are obtained by solving the CCSD left eigenvalue problem, referred in quantum chemistry to as the ‘lambda equations’). Similar equations can be given for two-body and higher-than-two-body reduced density matrices and properties.

An interesting feature of the EOMCCSD approach is the possibility to examine open-shell nuclei that are obtained by adding or removing one particle in a closed-shell system. This can be done by exploiting the particle-attached (PA) (in chemistry, electron-attached or EA) and particle-removed (PR) (in chemistry, ionized or IP) EOMCCSD approaches, in which we define the wavefunctions of the $(A + 1)$ - and $(A - 1)$ -particle systems as $|\Psi_\mu^{(A+1)}\rangle = (r_a a^a + \frac{1}{2} r_{ab}^j a^a a^b a_j) \exp(T_1 + T_2) |\Phi\rangle$ and $|\Psi_\mu^{(A-1)}\rangle = (r^i a_i + \frac{1}{2} r_b^{ij} a^b a_j a_i) \exp(T_1 + T_2) |\Phi\rangle$, respectively (see, e.g., [5, 31, 32]). The 1p and 2p-1h amplitudes r_a and r_{ab}^j , respectively, are obtained by diagonalizing the similarity transformed Hamiltonian \bar{H} obtained in the CCSD calculations for the closed-shell A -particle system in the $(A + 1)$ -particle sector of the Fock-space spanned by the $|\Phi^a\rangle = a^a |\Phi\rangle$ and $|\Phi_j^{ab}\rangle = a^a a^b a_j |\Phi\rangle$ determinants. Similarly, the 1h and 2h-1p amplitudes r^i and r_b^{ij} , respectively, are obtained by diagonalizing \bar{H} in the $(A - 1)$ -particle subspace spanned by $|\Phi_i\rangle = a_i |\Phi\rangle$ and $|\Phi_{ij}^b\rangle = a^b a_j a_i |\Phi\rangle$ determinants. We used the PA-EOMCCSD and PR-EOMCCSD methods, as defined above, to determine the binding and selected excitation energies of the ^{17}O and ^{15}O nuclei, using the similarity-transformed Hamiltonian \bar{H} obtained in the CCSD/EOMCCSD calculations for ^{16}O .

The CCSD and EOMCCSD methods capture the bulk of correlation effects with the inexpensive computational steps that scale as $n_o^2 n_u^4$, where $n_o(n_u)$ is the number of occupied (unoccupied) single-particle states, but there may be cases where three-body clusters T_3 and three-body components R_3 and L_3 become important. We can estimate the effects of T_3 and R_3 on ground- and excited-state energies by adding the *a posteriori* corrections to the CCSD and EOMCCSD energies E_μ , defining the CR-CCSD(T) and CR-EOMCCSD(T) approaches [8, 18, 22, 33], which require the relatively inexpensive $n_o^3 n_u^4$ non-iterative steps. We use the CR-CCSD(T) and CR-EOMCCSD(T) methods to examine T_3/R_3 effects on the energies of the ground and the lowest 3^- states of ^{16}O .

3. Discussion of the results

3.1. Ground-state energy calculations for ^{16}O

We begin our discussion with the results obtained for ^{16}O . As shown in table 2, we obtain a rapid convergence of the CCSD and CR-CCSD(T) ground-state energies of ^{16}O with the number of major oscillator shells (N), so that the results obtained with seven major oscillator shells are essentially converged. For example, the difference between the $N = 8$ and $N = 7$ CCSD/Idaho-A energies is only 0.5 MeV. We can also see that the triples (T_3) corrections to the ground-state CCSD energies, resulting from CR-CCSD(T) calculations, are small,

Table 2. The energies of the ground state and the lowest 3^- state obtained with the CCSD/EOMCCSD (abbreviated as SD) and CR-CCSD(T)/CR-EOMCCSD(T) (abbreviated as SD(T)) approaches, and $N = 5$ –8 major oscillator shells (in MeV), using the Idaho-A potential without Coulomb (ground state and the 3^- state) and N3LO potential (ground-state only). The starting-energy value was $\bar{\omega} = -80$ MeV.

N	Ground state (Idaho-A)		Ground state (N3LO)		The lowest 3^- state (Idaho-A)	
	SD	SD(T)	SD	SD(T)	SD	SD(T)
5	−125.92	−126.26	−108.94	−109.22	−112.35	−112.48
6	−121.53	−121.76	−113.34	−113.51	−108.55	−108.72
7	−120.16	−120.76	−112.45	−112.81	−108.20	−108.46
8	−119.62		−111.22			

contributing less than 1% of the total binding energy. This confirms our earlier findings for ^{16}O obtained with four major oscillator shells [18].

An extrapolation based on fitting the data in table 2 to $E(N) = E_\infty + a \exp(-b \cdot N)$, where the extrapolated energy E_∞ and a and b are parameters for the fit, shows that the extrapolated CCSD and CR-CCSD(T) energies obtained with the Idaho-A potential without Coulomb are -119.4 and -120.5 MeV, respectively. Coulomb adds to the binding approximately 11.2 MeV, so that our estimated Idaho-A ground-state energy, resulting from the CR-CCSD(T) calculations, is -109.3 MeV, compared to an experimental binding energy of -128 MeV. Our $N = 7$ ($N = 8$) N3LO CCSD and $N = 7$ CR-CCSD(T) energies, which include the Coulomb interactions, are -112.4 (-111.2) and -112.8 MeV, respectively, in excellent agreement with the Coulomb-corrected energies obtained with Idaho-A. We conclude that the two-body interactions underbind ^{16}O by approximately 1 MeV per particle, leaving room for the additional binding to be produced by three-body forces.

3.2. Calculations of the first excited 3^- state of ^{16}O

The first excited 3^- state of ^{16}O , located experimentally at 6.12 MeV above the ground state, is thought to be a $1p$ – $1h$ state [34]. The experience of quantum chemistry tells us that the EOMCCSD method describes $1p$ – $1h$ excited states almost exactly and that the triples (T_3 and R_3) effects on excitation energies of such states are negligible, provided that the three-body interactions in the Hamiltonian can be ignored. The largest R_1 amplitudes obtained in the EOMCCSD calculations for the 3^- state of ^{16}O indicate that the dominant $1p$ – $1h$ excitations are from the $0p_{1/2}$ orbital to the $0d_{5/2}$ orbital and that the $2p$ – $2h$ excitations in the EOMCCSD wavefunction, defined as $R_2 + R_1 T_1 + R_0(T_2 + T_1^2/2)$ ($R_0 = 0$ in this case), are much smaller than the R_1 amplitudes, confirming the $1p$ – $1h$ nature of the 3^- state. As expected, the CR-EOMCCSD(T) calculation hardly changes the total energy of the state. Our extrapolated Idaho-A results, employing the 3^- energies shown in table 2 and the same $E(N) = E_\infty + a \exp(-b \cdot N)$ fit as used in the ground-state case, indicate that the lowest 3^- state of ^{16}O lies at -108.2 and -108.4 MeV in the EOMCCSD and CR-EOMCCSD(T) calculations, respectively. Thus, the CR-EOMCCSD(T) method employing Idaho-A gives an excitation energy of 12.0 MeV for this state. The N3LO calculations (not shown in table 2) yield similar results. The ~ 6 MeV difference between the extrapolated CR-EOMCCSD(T) and experimental results suggests that the Idaho-A and N3LO potentials cannot yield an excitation energy for the 3^- state which would agree with experiment. Our results are converged at the coupled-cluster level employing the Idaho-A and N3LO two-body interactions, so that it

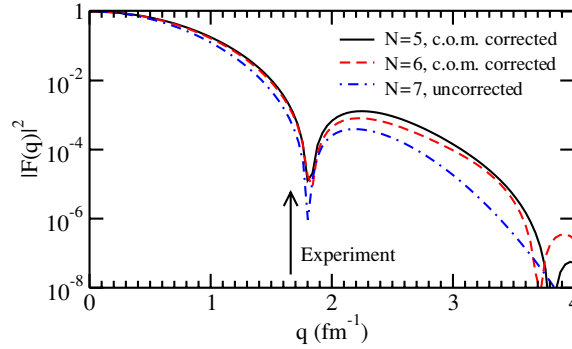


Figure 1. The charge form factor computed from the CCSD density matrix obtained with the Idaho-A potential.

(This figure is in colour only in the electronic version)

is possible that the discrepancy between theory and experiment resides in the Hamiltonian. We may have to include three-body forces to reduce the ~ 6 MeV difference between coupled-cluster and experimental excitation energies for the lowest 3^- state of ^{16}O .

3.3. One-body densities and charge form factor of ^{16}O

We also performed the CCSD calculations of the one-body reduced density matrices and the corresponding ground-state densities of ^{16}O using the recipe described in section 2.2. The resulting radial densities were used to determine the root-mean-square (rms) charge radii. After correcting for the finite sizes of the nucleons and the c.o.m. motion, we obtained the rms charge radii of 2.45, 2.50 and 2.51 fm for five, six and seven major oscillator shells, respectively, when the Idaho-A potential was employed, in good agreement with the experimental charge radius of ^{16}O of 2.73 ± 0.025 fm. The N3LO calculations gave similar values. We also calculated the nuclear charge form factor of ^{16}O , following the prescription described in [15, 16]. The form factor includes contributions due to the two-body reduced density matrix, resulting from the c.o.m. corrections, in addition to the contributions from the one-body density. We computed the one-body density contributions (for five, six and seven major oscillator shells) within the framework of CCSD theory precisely using the recipe described in section 2.2. The two-body density matrix, needed to correct the charge form factor for the c.o.m. terms (for five and six major oscillator shells) was calculated as $\rho_{pqrs} = \langle \Psi_0 | a^p a^q a_s a_r | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle$, where the CCSD ground-state wavefunction $|\Psi_0\rangle$ was approximated by the truncated shell-model-like expansion $(1 + C_1 + C_2) |\Phi\rangle$, with $C_1 = T_1$ and $C_2 = T_2 + T_1^2/2$ representing the 1p–1h and 2p–2h components of the CCSD wavefunction $\exp(T_1 + T_2) |\Phi\rangle$. The results of our calculations are shown in figure 1. As one can see, the c.o.m.-corrected charge form factors obtained with five and six major oscillator shells are very reasonable. Compared to experiment (the arrow in figure 1), the location of the first zero of the CCSD form factor is slightly shifted towards larger q values, which is consistent with an underestimated value of the rms charge radius obtained in CCSD calculations.

3.4. Binding and excitation energies of ^{15}O and ^{17}O

The results of the PR-EOMCCSD calculations for the ground-state of ^{15}O , CCSD calculations for the ground-state ^{16}O , and PA-EOMCCSD calculations for the ground-state of ^{17}O for

Table 3. Ground-state energies per particle for the ^{15}O , ^{16}O and ^{17}O nuclei obtained with PR-EOMCCSD, CCSD, and PA-EOMCCSD, respectively, $N = 5$ and 6 major oscillator shells, and N3LO, and the corresponding experimental values (in MeV).

N	^{15}O	^{16}O	^{17}O
5	−6.07	−6.81	−6.43
6	−6.25	−7.08	−6.80
Experiment	−7.46	−7.98	−7.75

five and six major oscillator shells and the N3LO potential are shown in table 3. Although we have to examine the convergence of our results with N , it is encouraging to see that the binding energies per particle resulting from inexpensive coupled-cluster calculations with six major oscillator shells are in reasonable agreement with experiment. The PR-EOMCCSD/CCSD/PA-EOMCCSD approaches underbind the three nuclei by about 1 MeV per particle, pointing to the need for three-body forces, but the relative binding energies of ^{15}O , ^{16}O , and ^{17}O obtained in coupled-cluster calculations are in very good agreement with experiment. For example, the difference between binding energies of ^{17}O and ^{16}O is 0.23 MeV per particle. The PA-EOMCCSD and CCSD ground-state energies of ^{17}O and ^{16}O resulting from the calculations with six major oscillator shells differ by 0.28 MeV per particle. We plan to extend these calculations to excited states of ^{15}O and ^{17}O , which may reveal useful information about three-nucleon interactions. Our preliminary PA-EOMCCSD calculations for the $1/2^+$ and $3/2^+$ states of ^{17}O , employing six major oscillator shells, locate these states at 0.13 and 6.03 MeV above the $5/2^+$ ground state, respectively. The analogous PR-EOMCCSD calculations for the $3/2^-$ state of ^{15}O locate this state at 6.60 MeV above the $1/2^-$ ground state.

4. Summary

We performed large-scale coupled-cluster calculations for ^{16}O and preliminary calculations for ^{15}O and ^{17}O . We showed that the ^{16}O ground state is accurately described by the basic CCSD approximation. The T_3 clusters contribute less than 1% of the binding energy. We attribute the 1 MeV per particle difference between the coupled-cluster and experimental binding energies to three-body forces. The ~ 6 MeV difference between the converged coupled-cluster results for the lowest 3^- state of ^{16}O and the corresponding experimental excitation energy is likely due to an inadequate description of the relevant nuclear forces by the two-body Idaho-A and N3LO Hamiltonians. The CCSD method provides a reasonable description of charge radius and charge form factor of ^{16}O . Finally, the PR-EOMCCSD and PA-EOMCCSD approximations provide reasonable results for the binding energies of ^{15}O and ^{17}O , although we need to examine the convergence of the PR-EOMCCSD and PA-EOMCCSD results with the basis set.

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