Benchmark calculations for ^{3}H, ^{4}He, ^{16}O, and ^{40}Ca with *ab initio* coupled-cluster theory

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(Received 11 July 2007; published 8 October 2007)

We present *ab initio* calculations for ^{3}H, ^{4}He, ^{16}O, and ^{40}Ca based on two-nucleon low-momentum interactions $V_{\mathrm{low}\,k}$ within coupled-cluster theory. For ^{3}H and ^{4}He, our results are within 70 and 10 keV of the corresponding Faddeev and Faddeev-Yakubovsky energies. We study in detail the convergence with respect to the size of the model space and the single-particle basis. For the heavier nuclei, we report practically converged binding energies and compare with other approaches.

DOI: 10.1103/PhysRevC.76.044305 PACS number(s): 21.10.Dr, 21.30.−x, 21.60.Gx, 31.15.Dv

I. INTRODUCTION

Ab initio few- and many-body methods have been used with great success to explore the structure of light nuclei based on microscopic two- and three-nucleon interactions. For nuclei with $A \lesssim 12$ nucleons, several techniques provide practically exact solutions to the nuclear many-body problem and have been benchmarked to agree within numerical uncertainties for the ^{4}He ground-state energy and radius obtained from the nucleon-nucleon (NN) Argonne v_8 potential [1]. These methods include Faddeev-Yakubovsky equations [2], variational approaches [3–6], the Green's function Monte Carlo (GFMC) method [7], the no-core shell model (NCSM) [8,9], and the effective interaction hyperspherical harmonics method [10,11]. Many of the above approaches are, however, restricted to the lightest nuclei.

In recent years, the coupled-cluster method [12,13] was reintroduced in nuclear physics as a tool for *ab initio* nuclear structure calculations [14–21]. Coupled-cluster theory is size extensive and scales rather gently with an increasing number of nucleons and with the size of the model space and therefore has the potential to extend the reach to medium-mass nuclei. In this article, we address the question of whether the coupled-cluster method is as precise for few-body systems as the well-established methods. Several findings suggest that this is indeed the case. Mihaila and Heisenberg performed a microscopic calculation of the electron scattering structure function for ^{16}O and found excellent agreement with experimental data. Their calculations are based on a particle-hole energy expansion of the cluster operator. More recent applications [16–21] follow the "standard" approach of coupled-cluster calculations from quantum chemistry [22–25]. In these calculations, several results for helium isotopes [17,20] were found to be in good agreement with exact diagonalizations in sufficiently small model spaces and with corresponding renormalized interactions. However, except in the recent study of three-nucleon forces (3NF) in coupled-cluster theory [21], this approach has never been compared in detail to well-established few-body methods in the larger model spaces that are needed for convergence with modern NN interactions. It is the purpose of this work to fill this gap in nuclear physics and to place the coupled-cluster method in the group of *ab initio* approaches.

This article is organized as follows. In Sec. II, we begin with a brief discussion of the coupled-cluster method, the low-momentum interactions, and the employed basis spaces. Our main results for ^{3}H and ^{4}He are presented in Sec. III and for ^{16}O and ^{40}Ca in Sec. IV. We conclude with a summary in Sec. V.

II. METHOD, INTERACTIONS, AND MODEL SPACES

A. Coupled-cluster method

Coupled-cluster theory was invented by Coester and Kümmel almost 50 years ago [12,13]. During the 1970s, this approach was further developed and was used in many applications in nuclear physics. The review by the Bochum group [26] summarizes the status of the field in 1978. From there onward, applications in nuclear physics were more of a sporadic nature [27]. This was most probably due to the difficulty of hard NN interactions and their strong short-range repulsion and short-range tensor force. Mihaila and Heisenberg employed coupled-cluster theory in the late 1990s [14]. Their work culminated in the precise computation of the electron scattering form factor for ^{16}O based on the Argonne v_{18} potential combined with leading contributions from 3NF [15].

Parallel to the field of nuclear physics, coupled-cluster theory saw its own career in *ab initio* quantum chemistry. After the pioneering works by Čížek [28,29], the theory has become one of the main workhorses in quantum chemistry [22–25]. The sheer number of applications and developments in that field *de facto* established a "standard" or "canonical" way for how the method is being used to solve quantum many-body problems. Reference [22] gives a summary of state-of-the-art coupled-cluster calculations in quantum chemistry.

Recently, coupled-cluster theory has seen a renaissance in nuclear physics starting with the calculations of Ref. [16]. This

approach differs from the one by Mihaila and Heisenberg as it employs coupled-cluster theory in the spirit of quantum chemistry and uses softer interactions. So far, the present approach has employed G matrices for the description of ground and excited states in ^{4}He [17] and ^{16}O [18], and for nuclei in the vicinity of ^{16}O [19]. The most recent calculations are based directly on low-momentum interactions $V_{\mathrm{low}\,k}$ [30,31], and the method has been developed to describe weakly bound and unbound helium isotopes within a Gamow-Hartree-Fock basis [20] and to include 3NF [21].

Within coupled-cluster theory, the ground state of a mass A nucleus is written as

$$|\psi\rangle = e^{\hat{T}}|\phi\rangle, \tag{1}$$

where $|\phi\rangle = \prod_{i=1}^{A} \hat{a}_i^\dagger|0\rangle$ is a single-particle product state and

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \cdots + \hat{T}_A \tag{2}$$

is a particle-hole (p-h) excitation operator with

$$\hat{T}_k = \frac{1}{(k!)^2} \sum_{i_1,\ldots,i_k;a_1,\ldots,a_k} t_{i_1\ldots i_k}^{a_1\ldots a_k} \hat{a}_{a_1}^\dagger \ldots \hat{a}_{a_k}^\dagger \hat{a}_{i_k} \ldots \hat{a}_{i_1}. \tag{3}$$

Here and in the following, $i, j, k, \ldots$ label occupied single-particle orbitals (as defined by the product state $|\phi\rangle$), whereas $a, b, c, \ldots$ refer to unoccupied orbitals.

We take the reference state $|\phi\rangle$ as our vacuum state and normal-order the Hamiltonian $\hat{H}$ with respect to this state. In practice, we restrict ourselves to the truncation $\hat{T} = \hat{T}_1 + \hat{T}_2$. This is the coupled-cluster singles and doubles (CCSD) approximation, and the coupled-cluster equations are given by

$$E = \langle\phi|\bar{H}|\phi\rangle, \tag{4}$$

$$0 = \langle\phi_i^a|\bar{H}|\phi\rangle, \tag{5}$$

$$0 = \langle\phi_{ij}^{ab}|\bar{H}|\phi\rangle. \tag{6}$$

Here $|\phi_{i_1\ldots i_n}^{a_1\ldots a_n}\rangle = \hat{a}_{a_n}^\dagger \ldots \hat{a}_{a_1}^\dagger \hat{a}_{i_1} \ldots \hat{a}_{i_n}|\phi\rangle$ is a np-nh excitation of the reference state $|\phi\rangle$, and

$$\bar{H} = e^{-\hat{T}} \hat{H} e^{\hat{T}} = (\hat{H}e^{\hat{T}})_c \tag{7}$$

is the similarity-transformed Hamiltonian (note that $\bar{H}$ is non-Hermitian). The last expression on the right-hand side of Eq. (7) indicates that only fully connected diagrams contribute to the construction. The CCSD Eqs. (5) and (6) determine the amplitudes t_i^a and t_{ij}^{ab} of the 1p-1h and the 2p-2h excitation cluster operators, respectively. Once these nonlinear equations are solved, the amplitudes can be inserted into Eq. (4) to determine the ground-state energy.

We remind the reader that an exact solution of the many-body problem would require us to employ the full excitation operator Eq. (2). Such a calculation is as expensive as a full diagonalization of the Hamiltonian and therefore impossible for medium-mass nuclei. CCSD is very efficient in the sense that it is a highly accurate approximation with the investment of a modest numerical effort that scales as $O(n_o^2 n_u^4)$ with the number n_o of occupied and the number n_u of unoccupied single-particle orbitals, respectively. The inclusion of the 3p-3h cluster operator $\hat{T}_3$ would further increase the accuracy of the method. However, such singles-doubles coupled cluster calculations including perturbative triples (CCSDT) come at the expense of $O(n_o^3 n_u^5)$ and, at present, are already prohibitively expensive compared to CCSD. For this reason, there is need for more approximate treatments of the full triples equations.

There are various approximations to the full CCSDT equations, and the most popular of these schemes is the CCSD(T) approach [32]. CCSD(T) includes diagrams at the CCSDT level that appear up to fifth order in perturbation theory. It is a noniterative approach because, typically, converged singles and doubles excitation amplitudes are used in the calculation of the triples energy correction. The CCSD(T) approximation is relatively inexpensive compared to CCSDT; no storage of triples amplitudes is required and the computational cost is a noniterative $O(n_o^3 n_u^4)$ step. There is also a family of iterative triples correction schemes known as CCSDT-n [33]. Their derivation is based on perturbation theory arguments,

$$\begin{aligned}
\mathrm{CCSDT}-1 \quad & 0 = \langle\phi_{ijk}^{abc}|(\hat{F}\hat{T}_3 + \hat{H}\hat{T}_2)_c|\phi\rangle, \\
\mathrm{CCSDT}-2 \quad & 0 = \langle\phi_{ijk}^{abc}|\left(\hat{F}\hat{T}_3 + \hat{H}\hat{T}_2 + \hat{H}\hat{T}_2^2/2\right)_c|\phi\rangle, \\
\mathrm{CCSDT}-3 \quad & 0 = \langle\phi_{ijk}^{abc}|(\hat{F}\hat{T}_3 + \hat{H}e^{\hat{T}_1+\hat{T}_2})_c|\phi\rangle, \\
\mathrm{CCSDT} \quad & 0 = \langle\phi_{ijk}^{abc}|(\hat{H}e^{\hat{T}_1+\hat{T}_2+\hat{T}_3})_c|\phi\rangle.
\end{aligned} \tag{8}$$

Here, $\hat{F}$ denotes the Fock operator (the one-body operator that results from the normal ordering of the Hamiltonian). All these approaches require the storage of the full triples amplitudes t_{ijk}^{abc} and are therefore computationally considerably more expensive than the CCSD(T) approach. However, for cases where the CCSD(T) scheme breaks down, one expects the CCSDT-n approaches to perform better. The latter approaches treat the triples corrections self-consistently and also involve the corrections

$$\langle\phi_i^a|(\hat{V}\hat{T}_3)_c|\phi\rangle, \tag{9}$$

$$\langle\phi_{ij}^{ab}|(\hat{F}\hat{T}_3 + \hat{V}\hat{T}_3 + \hat{V}\hat{T}_3\hat{T}_1)_c|\phi\rangle, \tag{10}$$

to Eqs. (5) and (6), respectively. These corrections thus modify the values of the amplitudes t_i^a and t_{ij}^{ab}.

B. Low-momentum interactions and model spaces

Nuclear interactions depend on the resolution scale at which details are probed and resolved. This resolution scale dependence is similar to scale and scheme dependences in parton distribution functions. As a result, nuclear interactions are defined by an effective theory for NN, $3N$, and many-nucleon interactions and corresponding effective operators,

$$\hat{V} = V_{NN}(\Lambda) + V_{3N}(\Lambda) + \cdots, \tag{11}$$

where the momentum cutoff Λ denotes the resolution scale. Conventional nuclear forces are "hard" in the sense that they have large cutoffs that complicate few- and many-body calculations. These difficulties arise from high momenta and associated strong short-range repulsion and short-range tensor forces, which lead to slow convergence with increasing basis size and requires resummations in practice.

Low-momentum interactions $V_{\mathrm{low}\,k}$ with variable momentum cutoffs show great promise for nuclei [30,31,34–39]. Changing the cutoff leaves low-energy NN observables unchanged by construction but shifts contributions between the potential and the sums over intermediate states in loop integrals. These shifts can weaken or largely eliminate sources of nonperturbative behavior such as strong short-range repulsion [35,40]. An additional advantage is that the corresponding $3N$ interactions become perturbative at lower cutoffs in $A = 3, 4$ nuclei [34], and are thus tractable in coupled-cluster theory [21]. The renormalization group (RG) evolution is implemented by coupled RG equations in momentum space [41] or by a corresponding Lee-Suzuki transformation [42–44] and subsequent implementations by Suzuki *et al*. [45].

The evolution to low-momentum interactions $V_{\mathrm{low}\,k}$ weakens off-diagonal coupling and decouples the low-energy physics from high-momentum details [46,47]. As a result, few- and many-body calculations converge more rapidly for lower cutoffs, which is important for extending *ab initio* approaches to heavier systems. Finally, the cutoff variation can provide estimates for theoretical uncertainties, which will be left to future work. In this article, we use a sharp cutoff $\Lambda = 1.9$ fm^{-1} for the ^{3}H and ^{4}He calculations, and $V_{\mathrm{low}\,k}$ is derived from the Argonne v_{18} potential [48] to benchmark against the Faddeev and Faddeev-Yakubovsky results [34]. For ^{16}O and ^{40}Ca, we use a cutoff $\Lambda = 2.1$ fm^{-1} and compare to the importance-truncated NCSM study [49].

Note that $3N$ interactions are important for the correct saturation properties of nuclei. Nuclear saturation is a many-body phenomenon and requires many-nucleon interactions. This is true for "hard" potentials (such as the Argonne v_{18} potential) and for "soft" low-momentum interactions. The main difference is that the former leads to underbinding in many-nucleon systems, whereas the latter leads to overbinding (for cutoffs around $\Lambda \sim 2$ fm^{-1}). Neither underbinding nor overbinding agrees with experiment, and $3N$ interactions are unavoidable for a correct description of nuclei.

Consistent $3N$ forces could be constructed by performing the RG evolution to low-momentum interactions in the two- and three-nucleon sector. Recall that the RG is an exact method. For instance, if the evolution starting from chiral EFT interactions were carried out in the NN and $3N$ sector, the RG would reproduce the same observables up to truncation errors in the EFT. However, the RG evolution of $3N$ forces has not yet been performed and is presently approximated by fitting the leading-order chiral $3N$ interactions [50,51] to $V_{\mathrm{low}\,k}$ for various cutoffs [34]. It has been checked in all applications that the resulting low-momentum 3N contributions are consistent with $\langle V_{3\mathrm{N}}\rangle \sim (Q/\Lambda)^3\langle V_{\mathrm{low}\,k}\rangle$, as expected from power-counting estimates [34,35,52]. This choice of $3N$ interactions with $V_{\mathrm{low}\,k}$ is well motivated because both approaches aim at a description of nuclei through low-momentum degrees of freedom. Nevertheless, in this work we will neglect $3N$ interactions and limit ourselves to low-momentum NN interactions. This is a significant simplification and allows us to perform our calculations in very large model spaces. We thus sacrifice saturation at the experimental energies and densities for the purpose of clean benchmark calculations that reach up to ^{40}Ca.

Coupled-cluster theory is employed in a single-particle basis, and we use a model space consisting of spherical harmonic-oscillator states. The basis parameters are the number of orbitals and the oscillator frequency $\hbar\omega$. Our largest model spaces include about 10^3 single-particle orbitals.

III. RESULTS FOR ^{3}H AND ^{4}HE

In this section, we present our coupled-cluster calculations for the ground-state energies of ^{3}H and ^{4}He, and we compare our results to the exact Faddeev and Faddeev-Yakubovsky energies of Ref. [34]. We first discuss in detail the dependence on the size of the model space and the single-particle basis. The coupled-cluster calculations initially used a single-particle basis of oscillator states whose principal and angular momentum quantum numbers n and l obey $2n + l \leqslant N$, so $N + 1$ is the number of major oscillator shells included. Note that in previous calculations [14–17] N denoted the number of major oscillator shells. However, we observed that the convergence with respect to the angular momentum l is much quicker, because only low partial waves contribute to low-energy properties, whereas the convergence with respect to the principal quantum number n is slower. This slower convergence is due to the sharp momentum cutoff used for $V_{\mathrm{low}\,k}$. It is intuitively clear that a harmonic-oscillator representation of an interaction with a sharp cutoff needs a considerable number of radial wave functions to be accurate. The recent work of Refs. [39,53] confirms this picture and demonstrates that smooth cutoffs improve the convergence in few-body calculations.

Figures 1 and 2 show the convergence of our CCSD and CCSD(T) energies for ^{3}H and ^{4}He using a model space with fixed $N = 2n + l = 12$ and fixed $\hbar\omega = 14$ MeV as a function of the maximum orbital angular momentum l. This implies that for $l = 0$ we include oscillator functions with $n \leqslant 6$ nodes; for $l \leqslant 1$ we include oscillator functions with $n \leqslant 6$ for the s states ($l = 0$) and $n \leqslant 5$ for the p states ($l = 1$), and so on. Clearly, the angular momentum quantum number needs not to

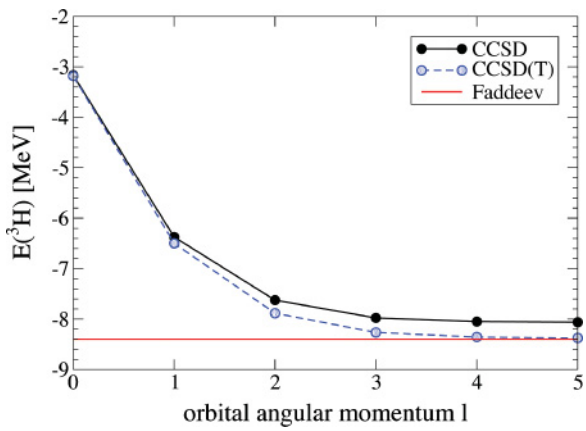

FIG. 1. (Color online) CCSD and CCSD(T) energies for ^{3}H using a model space with fixed maximum $N = 2n + l = 12$ and fixed $\hbar\omega = 14$ MeV as a function of the maximum orbital angular momentum l. For comparison, we also show the exact Faddeev result of Ref. [34].

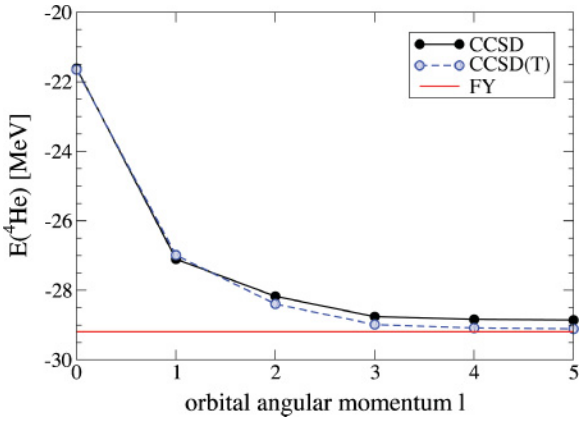

FIG. 2. (Color online) CCSD and CCSD(T) energies for ^{4}He as a function of the maximum orbital angular momentum l and the exact Faddeev-Yakubovsky (FY) result of Ref. [34]. For details, see the caption to Fig. 1.

exceed $l = 5$ for the ground-state energies of s-shell nuclei. Therefore, we limit our single-particle basis to $l \leqslant 5$ for the following coupled-cluster calculations of ^{3}H and ^{4}He.

In Figs. 3 and 4, we present our CCSD and CCSD(T) results for the ground-state energies of ^{3}H and ^{4}He as a function of the model-space size N, with fixed $l \leqslant 5$ and fixed $\hbar\omega = 14$ MeV. Both CCSD and CCSD(T) energies converge with respect to the model space size for $N \approx 12 \ldots 14$. For the largest model space with $N = 16$, we obtain for ^{3}H,

$$E_{\mathrm{CCSD}}(^3\mathrm{H}) = -8.09 \text{ MeV},$$
$$E_{\mathrm{CCSD(T)}}(^3\mathrm{H}) = -8.40 \text{ MeV},$$

and for ^{4}He,

$$E_{\mathrm{CCSD}}(^4\mathrm{He}) = -28.92 \text{ MeV},$$
$$E_{\mathrm{CCSD(T)}}(^4\mathrm{He}) = -29.18 \text{ MeV}.$$

The CCSD(T) energies are within 70 and 10 keV of the Faddeev and Faddeev-Yakubovsky (FY) results [34] $E(^3\mathrm{H}) = -8.470(2)$ MeV and $E(^4\mathrm{He}) = -29.19(5)$ MeV.

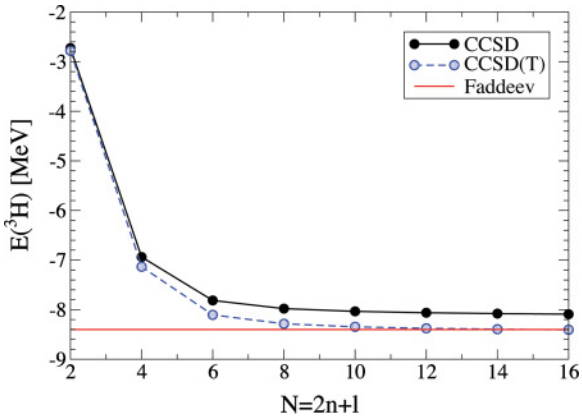

FIG. 3. (Color online) CCSD and CCSD(T) results for the ground-state energy of ^{3}H as a function of the model-space size $N = 2n + l$, with fixed $l \leqslant 5$ and fixed $\hbar\omega = 14$ MeV. For comparison, we also show the exact Faddeev result of Ref. [34].

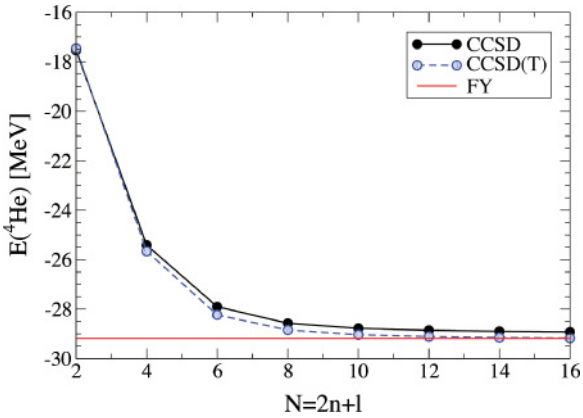

FIG. 4. (Color online) CCSD and CCSD(T) results for the ground-state energy of ^{4}He as a function of the model-space size $N = 2n + l$ and the exact Faddeev-Yakubovsky (FY) result of Ref. [34]. For details, see the caption to Fig. 3.

Finally, we study the dependence of our results on the oscillator frequency $\hbar\omega$. This is shown in Fig. 5 for fixed $N = 12$ and $l \leqslant 5$. Although the CCSD results exhibit a very small variation over the shown $\hbar\omega$ range, the variation of the perturbative triples corrections CCSD(T) is somewhat larger. Moreover, the downward trend of the CCSD(T) energies with decreasing $\hbar\omega$ indicates that perturbative triples corrections are starting to break down for smaller values of $\hbar\omega$. The noniterative perturbative triples correction assumes that we work in a basis where the Fock matrix is diagonal. However, our oscillator basis does not diagonalize the Fock matrix, so strict calculations would have to iterate triples corrections until self-consistency is reached. From Fig. 5 we observe that iterative CCSD(T) improves on the noniterative CCSD(T) results, but also has a downward trend with decreasing $\hbar\omega$. Finally, we present calculations based on the iterative CCSDT-1 approximation to full CCSDT. CCSDT-1 includes all diagrams through fourth order in perturbation theory, but contrary to the perturbative CCSD(T) corrections, the CCSDT-1 approximation is treated self-consistently and the singles and doubles amplitudes are modified by the triples

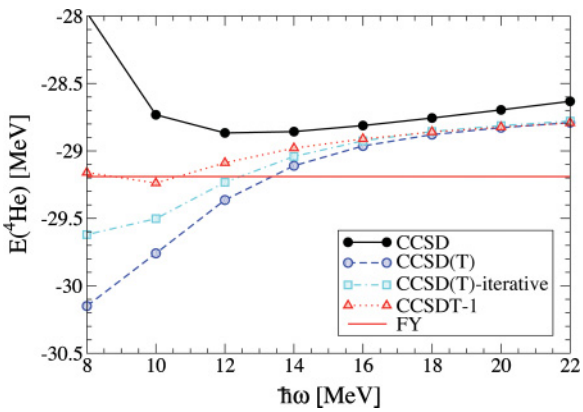

FIG. 5. (Color online) CCSD and various approximate CCSDT energies for ^{4}He as a function of the oscillator frequency $\hbar\omega$, for fixed $N = 12$ and $l \leqslant 5$. For comparison, we also show the exact Faddeev-Yakubovsky (FY) result.

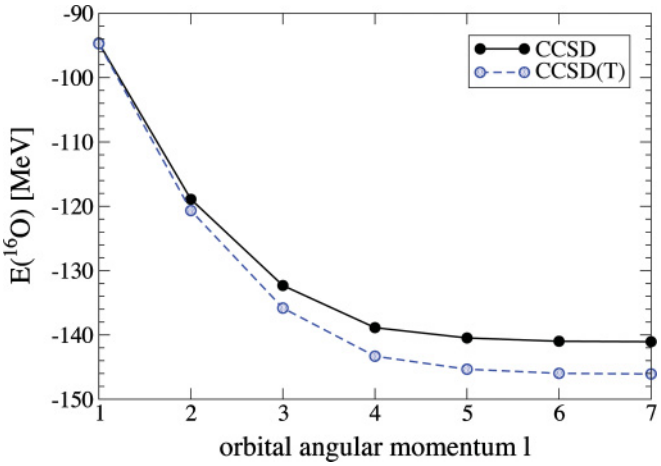

FIG. 6. (Color online) CCSD and CCSD(T) results for the binding energy of ^{16}O using a model space with fixed maximum $N = 2n + l = 10$ and fixed $\hbar\omega = 20$ MeV as a function of the maximum orbital angular momentum l.

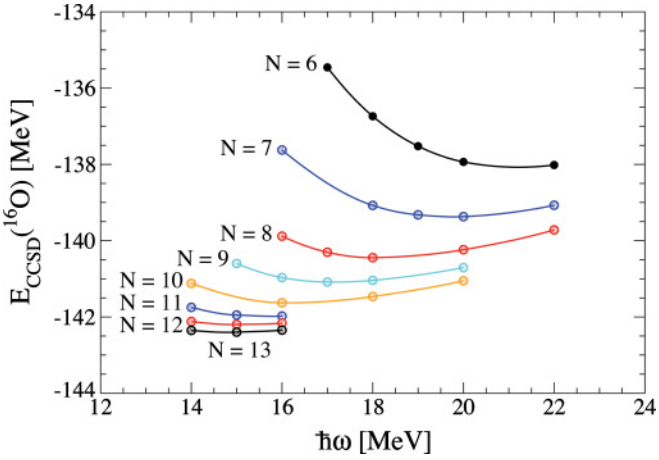

FIG. 7. (Color online) CCSD results for the binding energy of ^{16}O as a function of the oscillator frequency $\hbar\omega$ for increasing sizes of the model space $N = 2n + l$ with fixed $l \leqslant 7$.

amplitude according to Eqs. (9) and (10). We clearly find that CCSDT-1 improves on the triples corrections and leads to a very weak dependence on $\hbar\omega$. Note that these CCSDT-1 results are also the first step toward full CCSDT calculations in nuclear physics.

Our results for the light nuclei ^{3}H and ^{4}He demonstrate that coupled-cluster theory meets the benchmarks set by exact methods. It is therefore interesting to use this method to establish benchmark energies for heavier nuclei that other *ab initio* approaches can compare to. This is the subject of the next section.

IV. RESULTS FOR ^{16}O AND ^{40}Ca

Next, we present our coupled-cluster calculations for ^{16}O and ^{40}Ca. In Fig. 6, we show the convergence of the CCSD and CCSD(T) results for the binding energy of ^{16}O using a model space with fixed $N = 2n + l = 10$ and fixed $\hbar\omega = 20$ MeV as a function of the maximum orbital angular momentum l. For ^{16}O, we find that $l \leqslant 7$ is sufficient to reach convergence at the 10-keV level. Therefore, we restrict the following coupled-cluster calculations for ^{16}O to $l \leqslant 7$.

Figure 7 shows the dependence of the CCSD binding energies of ^{16}O on the oscillator frequency $\hbar\omega$ for increasing sizes of the model space N with fixed $l \leqslant 7$. The largest calculations for $N = 13$ include more than 10^3 single-particle orbitals. We observe that the CCSD energies are converged at the 0.5-MeV level and can be used to extrapolate to infinite model space. This is demonstrated in Fig. 8 where we give the CCSD energies (taken at the $\hbar\omega$ minima) as a function of the model-space size N at fixed $l \leqslant 7$. Using the CCSD minima, we make an exponential fit of the form $E(N) = E_\infty + a \exp(-bN)$ to the data points. The result is also shown in Fig. 8 and yields the extrapolated infinite model space value $E_{\mathrm{CCSD},\infty}(^{16}\mathrm{O}) = -142.78$ MeV. Our largest $N = 13$ result is $E_{\mathrm{CCSD}}(^{16}\mathrm{O}) = -142.40$ MeV. The conservative error estimate due to the finite size of the model space is thus about 0.5 MeV.

In Fig. 9, we study triples corrections to the binding energy of ^{16}O via the CCSD(T) and CCSDT-1 approaches as a function of the oscillator frequency $\hbar\omega$ for increasing sizes of the model space N ($l \leqslant 7$). We present results up to $N = 7$ (eight major oscillator shells), which was the largest model space we could handle for the CCSDT-1 scheme due to storage limitations. The CCSD(T) and CCSDT-1 energies agree nicely for the range of oscillator frequencies and model spaces considered. The only difference is that, as for ^{4}He, the CCSD(T) approach gives slightly more binding than CCSDT-1 for the largest model spaces. The close agreement between CCSD(T) and CCSDT-1 gives us confidence that the perturbative triples corrections work well over this regime.

Let us study the contributions of the triples amplitudes to the binding energy of ^{16}O in more detail. Figure 10 shows the energy differences $\Delta E = E - E_{\mathrm{CCSD}}$ that are

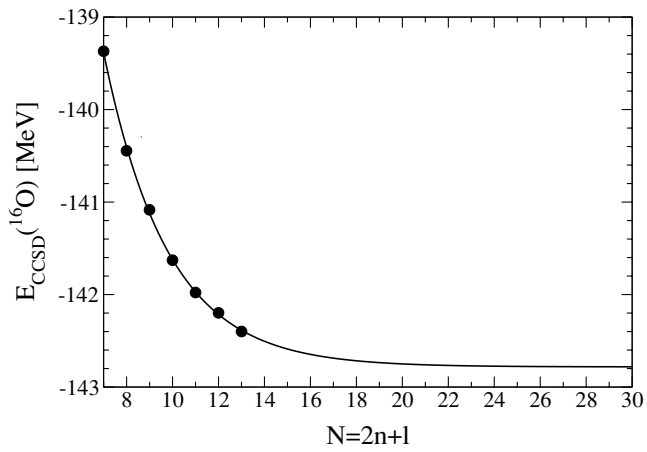

FIG. 8. CCSD results (taken at the $\hbar\omega$ minima) for the binding energy of ^{16}O as a function of the model-space size $N = 2n + l$ at fixed $l \leqslant 7$ and exponential fit (solid line).

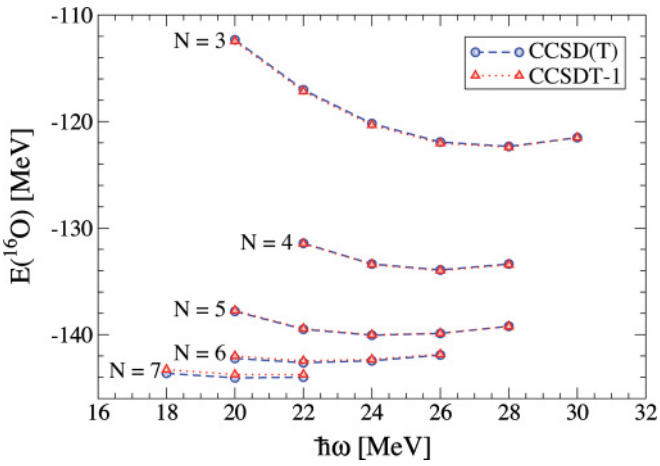

FIG. 9. (Color online) CCSD(T) and CCSDT-1 results for the binding energy of ^{16}O as a function of the oscillator frequency $\hbar\omega$ for increasing sizes of the model space $N = 2n + l$ ($l \leqslant 7$).

due to triples corrections "(T)" and "$T - 1$" as a function of the model-space size N at fixed $\hbar\omega = 22$ MeV and $l \leqslant 7$. The corresponding exponential extrapolations to infinite model spaces yield -5.45 MeV from the (T) correction and -5.00 MeV from the $T - 1$ correction. This suggests that the error estimate for the CCSD(T) and CCSDT-1 calculations is about 0.5 MeV. This can be viewed as an error estimate due to the truncation of the cluster operator. Combined with the 0.5 MeV uncertainty due to the size of the model space, we thus arrive at an error estimate of about 1 MeV for ^{16}O.

We note that ^{16}O is overbound by about 20 MeV when compared to the experimental binding energy. A similar result has been found by Fujii *et al.* [54]. However, a comparison of results based only on NN interactions to experiment is meaningless, because 3NF are crucial to describe few- and many-body observables (see, for instance, the discussion in Refs. [21,34,35]). In nuclear matter, the corresponding 3NF

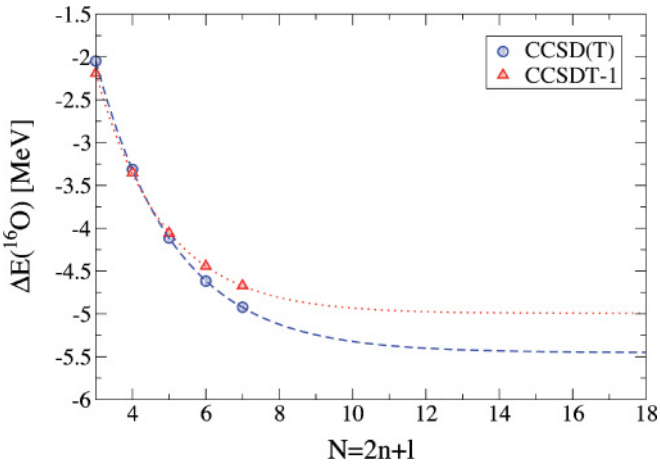

FIG. 10. (Color online) Contributions to the binding energy of ^{16}O from triples corrections CCSD(T) and CCSDT-1 as a function of the model-space size $N = 2n + l$ at fixed $\hbar\omega = 22$ MeV and $l \leqslant 7$. The dashed and dotted lines are exponential fits and yield the extrapolated energy corrections.

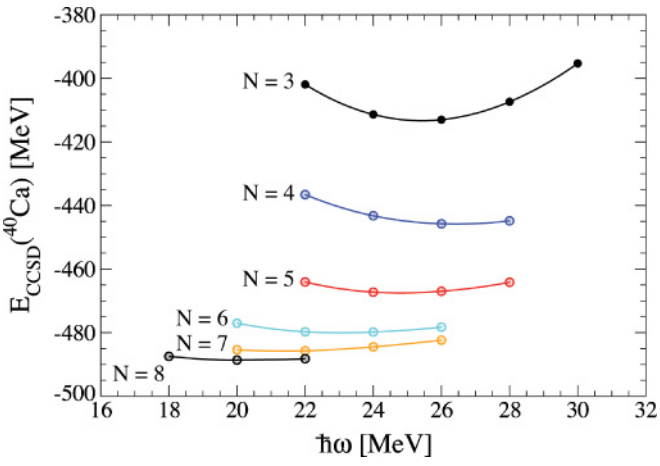

FIG. 11. (Color online) CCSD results for the binding energy of ^{40}Ca as a function of the oscillator frequency $\hbar\omega$ for increasing sizes of the model space $N = 2n + l$. (Note that there is no restriction on l for these model spaces.)

contribution is repulsive and the expectation values remain consistent with chiral effective field theory power-counting estimates [35].

Finally, we turn to the more challenging case of ^{40}Ca. Figure 11 shows the CCSD binding energy of ^{40}Ca as a function of the oscillator frequency $\hbar\omega$ for model spaces up to $N = 8$ (nine major oscillator shells). (Note that there is no restriction on l for these model spaces.) This represents the largest coupled-cluster calculation to date in nuclear physics. In these largest calculations, we have 40 active particles in 660 single-particle orbitals. The effective shell-model dimension in this space would be of the order of 10^{63}. From Fig. 11, we find that the CCSD energies of ^{40}Ca are converging reasonably well. We again expect that low-momentum interactions with smooth cutoffs will lead to even improved convergence. In Fig. 12, we present the CCSD energies for ^{40}Ca (taken at the $\hbar\omega$ minima) as a function of the model-space size N.

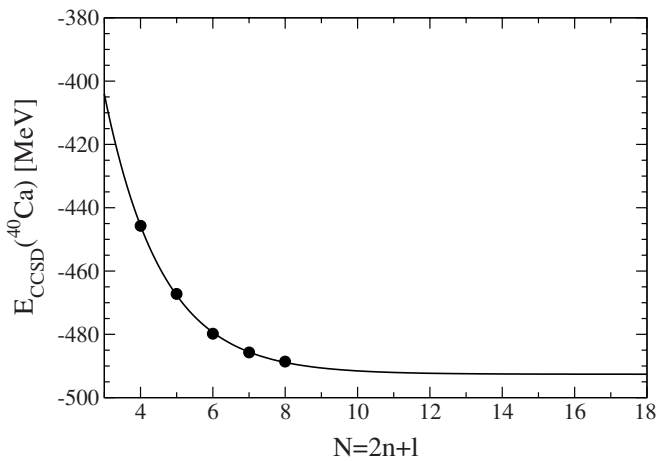

FIG. 12. CCSD results (taken at the $\hbar\omega$ minima) for the binding energy of ^{40}Ca as a function of the model-space size $N = 2n + l$ (without restriction in l) and exponential fit (solid line).

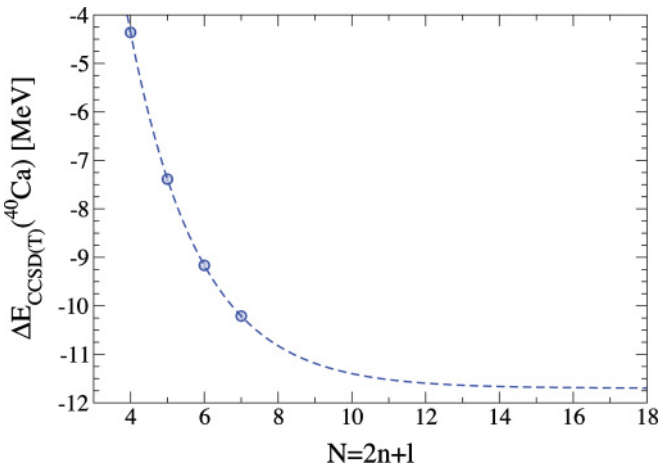

FIG. 13. (Color online) Contributions to the binding energy of ^{40}Ca from triples corrections CCSD(T) as a function of the model-space size $N = 2n + l$ at fixed $\hbar\omega = 22$ MeV (without restriction in l) and exponential fit (dashed line).

The exponential extrapolation to infinite model space yields $E_{\mathrm{CCSD},\infty}(^{40}\mathrm{Ca}) = -492.6$ MeV, and we find that the CCSD energy for $N = 8$ is about 4 MeV from the fully converged CCSD result.

We then perform CCSD(T) calculations and show in Fig. 13 the triples energy corrections as a function of the model-space size N at fixed $\hbar\omega = 22$ MeV. Due to memory limitations, we were not able to perform CCSDT-1 calculations in model spaces reaching up to $N = 7$. The exponential extrapolation to infinite model space yields -11.70 MeV, whereas the largest $N = 7$ result is -10.21 MeV. The convergence we find with respect to the size of the model space is similar to the recent results by Fujii *et al.* [55]. Recall that the different triples corrections for ^{16}O differed by about 10% from each other. Thus, we estimate that the error due to the truncation of the cluster operator is about 1 MeV for ^{40}Ca. The total error estimate for ^{40}Ca is thus about 5 MeV and is dominated by the uncertainty due to the finite size of the model space.

We summarize our coupled-cluster results for the binding energies of ^{4}He, ^{16}O, and ^{40}Ca in Table I, which gives the extrapolated correlation energies ΔE_{CCSD} and $\Delta E_{\mathrm{CCSD(T)}}$. We find that for ^{4}He, ^{16}O, and ^{40}Ca, the triples corrections are a factor of $\approx$0.015, 0.066, and 0.081 smaller than the CCSD correlation energies. From this, we again estimate the missing correlation energy from quadruples, pentuplets, and so on, to be of the order of 1 MeV for ^{40}Ca. We note that ^{16}O is overbound by about 20 MeV and ^{40}Ca by about 150 MeV when compared to the experimental binding energies. This is not surprising and points to the importance of 3NF for nuclear structure calculations [21,34,35].

TABLE I. Reference vacuum energies, E_0, CCSD, and CCSD(T) correlation energies, ΔE_{CCSD} and $\Delta E_{\mathrm{CCSD(T)}}$, and binding energies $E_{\mathrm{CCSD(T)}}$ for ^{4}He, ^{16}O, and ^{40}Ca. The vacuum energies, E_0, are for $\hbar\omega = 14$ MeV in the case of ^{4}He and $\hbar\omega = 22$ for ^{16}O and ^{40}Ca. The CCSD and CCSD(T) energies are the extrapolated infinite model space results. The exact Faddeev-Yakubovsky result is from Ref. [34].

	^{4}He	^{16}O	^{40}Ca
E_0	−11.8	−60.2	−347.5
ΔE_{CCSD}	−17.1	−82.6	−143.7
$\Delta E_{\mathrm{CCSD(T)}}$	−0.3	−5.4	−11.7
$E_{\mathrm{CCSD(T)}}$	−29.2	−148.2	−502.9
Exact (FY)	−29.19(5)		

We can compare the coupled-cluster energies to the recent importance-truncated NCSM results of Roth and Navrátil [49] which are based on the same $V_{\mathrm{low}\,k}$ interaction. The importance-truncated NCSM combines a particle-hole truncation scheme (4p-4h for ^{16}O and 3p-3h for ^{40}Ca in Ref. [49]) with importance sampling of many-body states based on perturbation theory. The particle-hole truncation scheme leads to unlinked diagrams and hence is not size extensive [22]. Using an exponential extrapolation, Roth and Navrátil [49] find binding energies $E = -137.75$ MeV for ^{16}O and $E = -461.83$ MeV for ^{40}Ca at the minimum in $\hbar\omega$. Our coupled-cluster results indicate that the converged energies are approximately 10 and 40 MeV lower for ^{16}O and ^{40}Ca, respectively. Note also that CCSD scales computationally more favorably than a full 4p-4h calculation, whereas it already includes a considerable part of linked 4p-4h excitations [22].

V. SUMMARY

In summary, we have performed *ab initio* coupled-cluster calculations for ^{3}H, ^{4}He, ^{16}O, and ^{40}Ca based on low-momentum interactions $V_{\mathrm{low}\,k}$. At the CCSD(T) level, the ground-state energies for ^{3}H and ^{4}He are practically converged with respect to the size of the model space and exhibit a very weak dependence on the oscillator frequency. The resulting energies are within 70 and 10 keV of the corresponding Faddeev and Faddeev-Yakubovsky benchmarks. For ^{16}O and ^{40}Ca, we estimate that the CCSD(T) binding energies are converged within 1 and 5 MeV, respectively. Future calculations will include convergence studies for low-momentum interactions with smooth cutoffs [46,53] and advancing the 3NF frontier to medium-mass nuclei based on the findings of Ref. [21]. Our results confirm that coupled-cluster theory is a powerful *ab initio* method that meets and sets benchmarks.

ACKNOWLEDGMENTS

We thank S. K. Bogner, R. J. Furnstahl, and A. Nogga for useful discussions. This work was supported by the U.S. Department of Energy under contract nos. DE-AC05-00OR22725 with UT-Battelle, LLC (Oak Ridge National Laboratory), and DE-FC02-07ER41457 (University of Washington), and under grant no. DE-FG02-96ER40963 (University of Tennessee), and by the Natural Sciences and Engineering Research Council of Canada (NSERC). TRIUMF receives federal funding via a contribution agreement through the National Research Council of Canada. Computational resources were provided by the National Center for Computational Sciences at Oak Ridge and the National Energy Research Scientific Computing Facility.

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