Ab initio coupled-cluster and configuration interaction calculations for ^{16}O using the V_{UCOM} interaction

Robert Roth*
Institut für Kernphysik, Technische Universität Darmstadt, D-64289 Darmstadt, Germany

Jeffrey R. Gour and Piotr Piecuch†
Department of Chemistry, Michigan State University, East Lansing, Michigan 48824-1322, USA
(Received 30 May 2008; revised manuscript received 7 November 2008; published 21 May 2009)

Using the ground-state energy of ^{16}O obtained with the realistic V_{UCOM} interaction as a test case, we present a comprehensive comparison of different configuration interaction (CI) and coupled-cluster (CC) methods, analyzing the intrinsic advantages and limitations of each of the approaches. In particular, we use the importance-truncated (IT) CI and no-core shell model (NCSM) schemes with up to 4-particle-4-hole (4p4h) excitations, with and without the Davidson extensivity corrections, as well as the size extensive CC methods with a complete treatment of one- and two-body clusters (CCSD) and a noniterative treatment of connected three-body clusters via the completely renormalized correction to the CCSD energy defining the CR-CC(2,3) approach, which are all capable of handling larger systems with dozens of explicitly correlated fermions. We discuss the impact of the center-of-mass contaminations, the choice of the single-particle basis, and size-extensivity on the resulting energies. When the IT-CI and IT-NCSM methods include the 4p4h excitations and when the CC calculations include the 1p1h, 2p2h, and 3p3h clusters, as in the CR-CC(2,3) approach, we observe an excellent agreement among the different methodologies, particularly when the Davidson extensivity corrections are added to the IT-CI energies and the effects of the connected three-body clusters are accounted for in the CC calculations. This shows that despite their individual limitations, the IT-CI, IT-NCSM, and CC methods can provide precise and consistent *ab initio* nuclear structure predictions. Furthermore, the IT-CI, IT-NCSM, and CC ground-state energy values obtained for ^{16}O are in reasonable agreement with the experimental value, providing further evidence that the V_{UCOM} two-body interaction may allow for a good description of binding energies for heavier nuclei and that all of the methods used in this study account for most of the relevant particle correlation effects.

DOI: 10.1103/PhysRevC.79.054325 PACS number(s): 21.60.Cs, 21.60.De, 31.15.bw, 27.20.+n

I. INTRODUCTION

Recent developments in nuclear structure theory have lead to new perspectives for a QCD-based *ab initio* description of *p*-shell nuclei and beyond. Significant advances have been made regarding the two main ingredients for an *ab initio* treatment of nuclear structure: the realistic interaction defining the relevant Hamiltonian and the solution of the quantum many-body problem. In addition to traditional realistic interactions, including the Argonne V18 [1] or the CD Bonn potential [2], the framework of chiral effective field theory [3,4] has been used to construct consistent two- and many-nucleon interactions based on the relevant degrees of freedom and the symmetries of QCD [5–7].

Based on these bare interactions, several methods have been developed to adapt the nuclear Hamiltonian to the limited model spaces available in practical many-body calculations. Different conceptual frameworks ranging from the $V_{\mathrm{low}k}$ renormalization group method [8] and the similarity renormalization group scheme [9–11] to the unitary correlation operator method [12–15] are being used to construct soft, phase-shift equivalent interactions, which exhibit superior convergence properties when employed in many-body calculations.

Bare or transformed interactions are the starting point for modern computational approaches for the *ab initio* solution of the nuclear many-body problem. Two methods have become particularly successful in this area, namely the Green's function Monte Carlo approach [16–20] and the no-core shell model [21–41]. For nuclei up to $A \approx 12$, detailed studies of ground and low-lying excited states, including detailed spectroscopic information, were conducted with both methods using different two-nucleon interactions and phenomenological three-nucleon forces. Very recently, the first *ab initio* no-core shell model calculations using the chiral two- plus three-nucleon interactions have shown the great potential that this new category of interactions may offer [38].

Although the Green's function Monte Carlo and no-core shell model approaches are successful in describing nuclei up to the mid-*p*-shell region, very few methods can provide a computationally tractable *ab initio* description of nuclei such as ^{16}O or beyond. Among those are the importance-truncated no-core shell model and the related importance-truncated configuration interaction methods and the coupled-cluster approach, which have recently been used for nuclear structure calculations in the $A = 16$ and $A = 40$ mass regions [39,42–52]. Extension of these methods toward heavier nuclei is presently in progress, within both the *ab initio* description and the traditional effective Hamiltonian approach (cf. Refs. [53,54]).

The coupled-cluster and configuration interaction methodologies that have been used in these recent developments are

*robert.roth@physik.tu-darmstadt.de
†piecuch@chemistry.msu.edu

complementary regarding their respective advantages and limitations. This work aims at a direct and quantitative comparison of the results of large scale *ab initio* importance-truncated configuration interaction, importance-truncated no-core shell model, and coupled-cluster calculations based on the same realistic Hamiltonian using the example of the ^{16}O ground state. We focus on the most practical coupled-cluster and configuration interaction approaches that have been specifically designed to handle larger systems with dozens of correlated particles and larger single-particle basis sets. The most essential formal differences, advantages, and limitations of the importance-truncated configuration interaction, importance-truncated no-core shell model, and coupled-cluster methods are addressed and their relevance for practical nuclear structure calculations is discussed. The nucleon-nucleon interaction used in this work is the V_{UCOM} potential derived in the unitary correlation operator method (UCOM) [12–15].

Following a description of the importance-truncated configuration interaction and coupled-cluster methods in Sec. II and III, we discuss the benchmark results for ^{16}O in Sec. IV. We assess in detail the impact of center-of-mass contaminations and the role of the single-particle basis and compare the results of large-scale calculations based on the importance-truncated configuration interaction, importance-truncated no-core shell model, and coupled-cluster methodologies with one another and with experiment.

II. IMPORTANCE-TRUNCATED CONFIGURATION INTERACTION

As a first class of methods, we consider different configuration interaction (CI) approaches. The common element of all CI methods, which are frequently used in nuclear structure theory and quantum chemistry, is that the eigenvalue problem for the Hamiltonian is solved in a many-body basis of Slater determinants or symmetry-adapted configuration state functions constructed from a given single-particle basis. In particular, the so-called full CI approach of quantum chemistry employs a model space spanned by all possible Slater determinants built from a finite set of single-particle orbits, providing the exact solution of the Schrödinger equation in that single-particle basis. Unfortunately, the dimension of the full CI model space grows factorially with the numbers of particles and single-particle orbits, limiting full CI calculations to small systems and relatively small single-particle basis sets.

Truncated CI models offer a simple and natural way of reducing the dimension of the model space and the prohibitive costs of full CI calculations. In the simplest scheme that defines the single-reference truncated CI models, only the excited determinants up to and including m-particle–m-hole (mpmh) excitations from the reference determinant $|\Phi_0\rangle$, where m is typically much smaller than the number of active particles, are included in the Hamiltonian diagonalization. By introducing the kpkh excitation operators C_k, the ground state emerges then as

$$|\Psi_0\rangle = \sum_{k=0}^{m} C_k\,|\Phi_0\rangle, \tag{1}$$

where $C_0\,|\Phi_0\rangle$ is the reference determinant contribution to $|\Psi_0\rangle$ and the $C_k\,|\Phi_0\rangle$ terms with $k = 1, \ldots, m$ are the kpkh components of the wave function included in the calculations. The popular approaches in this category of methods include CISD (CI singles and doubles), CISDT (CI singles, doubles, and triples), and CISDTQ (CI singles, doubles, triples, and quadruples), if we use the quantum-chemistry acronyms, or CI(mpmh) with $m = 2$, 3, and 4, respectively, if we use the particle-hole language of many-body physics. Because these truncated CI methods lack size extensivity (i.e., unlinked diagrams are present in the truncated CI wave function expansions, resulting in a potential loss of accuracy as the system becomes larger), the Davidson extensivity corrections [55] are usually added to the resulting energies to alleviate the problem.

Another popular scheme to define truncated CI models, which is frequently used in quantum chemistry and which is related to the importance-truncated nuclear CI methods considered in this work, is to consider the 1p1h and 2p2h excitations from the multiconfigurational reference space spanned by a number of determinants that provide a reasonable zero-order description of the many-body state or states of interest, as in the multireference CI methods [56,57]. The multireference CI approaches are particularly useful when a single reference determinant is a poor approximation to the eigenstate(s) of interest and when one wants to accelerate convergence toward the results of the exact diagonalization by selecting the dominant contributions to the wave function due to 3p3h, 4p4h, and other higher-order excitations. With the judicious choice of the multideterminantal reference state, the multireference CI methods can be very accurate, but they often lead to long wave-function expansions. Thus, to further reduce computer costs of multireference CI calculations, one often considers reduced sets or subsets of the resulting many-body basis states, which are usually defined through the internal contractions of configuration state functions or the multiconfigurational perturbation theory analysis coupled with numerical thresholds to reject unimportant configurations. The importance-truncation scheme used in this work uses similar ideas to those exploited in the multireference CI approaches, while enabling one to incorporate the higher-order mpmh excitations from the multideterminantal reference space in a systematic fashion. Again, because the multireference CI methods lack size extensivity, the multireference generalizations of the Davidson extensivity correction [57–61] are usually added to the resulting energies (for the alternative, more intrinsic ways of approximately restoring size extensivity in multireference CI calculations, see, e.g., Ref. [62] and references therein).

In nuclear structure theory, the CI concept is widely used in the form of the diagonalization shell model and all of its variants (see Ref. [41] and references therein). We consider only no-core calculations in this work, i.e., all particles are active. A full CI calculation would use a complete model space spanned by all Slater determinants that one can obtain for a given finite set of single-particle states, e.g., the harmonic-oscillator single-particle states up to a maximum principal quantum number $e_{\max}$, where $e = 2n + l$, with n and l representing the radial and angular-momentum quantum

numbers, respectively. Other finite sets of single-particle states, e.g., those extracted from a self-consistent Hartree-Fock calculation, can be employed in the CI calculations as well. The nuclear truncated CI(mpmh) approaches, where $m < A$, emerge then by considering the suitable subsets of Slater determinants from the full CI model space, including the reference determinant $|\Phi_0\rangle$ and all kpkh excitations from $|\Phi_0\rangle$ with $k = 1, \ldots, m$, as described above. By systematically increasing m, one approaches the full CI limit in which $m = A$, and by considering the $e_{\max} \to \infty$ limit, one approaches the exact solution of the Schrödinger equation for a given Hamiltonian. In the following, we will reserve the term CI exclusively for the diagonalization shell-model calculations based on this specific form of the single-particle truncation.

A modification of the above full and truncated CI methods, which has been used in several highly successful *ab initio* investigations of nuclei in recent years, is the no-core shell model (NCSM) [21–41]. The NCSM formalism uses a different definition of the complete model space than that employed in full CI. Instead of considering all Slater determinants that one can obtain for a given set of the harmonic-oscillator single-particle states up to a maximum principal quantum number $e_{\max}$, in the NCSM approach one includes those Slater determinants with an unperturbed excitation energy that does not exceed $N_{\max}\hbar\Omega$, where Ω is the frequency associated with the harmonic oscillator basis [21–41]. The exact solution of the Schrödinger equation for a given Hamiltonian is systematically approached by considering the $N_{\max} \to \infty$ limit. Although the NCSM calculations rely on the general CI concept of the diagonalization of the Hamiltonian used in all shell-model calculations, in this work we distinguish between methods that employ all or some Slater determinants resulting from the truncation of the single-particle space, which we continue calling the CI methods, and the NCSM approaches that represent the special type of shell-model calculations which uses the $N_{\max}\hbar\Omega$ model spaces. Typically, for the reasons explained below, the NCSM calculations are performed in the harmonic-oscillator bases (cf., however, Ref. [30] for the Hartree-Fock based NCSM study).

For the application to nuclei, the NCSM model spaces offer a few important advantages over the model spaces used in CI calculations. Unlike in quantum chemistry, where the issue of center-of-mass does not exist due to the Born-Oppenheimer approximation, the proper description of self-bound nuclei requires that special care is taken regarding the center-of-mass contamination of intrinsic states. Only the NCSM model spaces, in which the cutoff for the Slater determinants included in the calculations is defined by setting up the maximum unperturbed excitation energy at $N_{\max}\hbar\Omega$, allow for an exact separation of intrinsic and center-of-mass motions, which is necessary to obtain translationally invariant intrinsic states, as long as a harmonic-oscillator single-particle basis is used. The CI truncations, in which the cutoff for the Slater determinants included in the calculations is typically defined by the number of major harmonic oscillator shells corresponding to the maximum principal quantum number $e_{\max}$, as defined above, violate the separation of intrinsic and center-of-mass motions, resulting in the center-of-mass contaminated states. The degree of center-of-mass contamination goes down as $e_{\max} \to \infty$ and $m \to A$, but one cannot eliminate it mathematically, as in the NCSM case. Furthermore, the truncation with respect to the unperturbed excitation energy used in the NCSM calculations automatically identifies the most relevant Slater determinants in the wave function expansion, as is clear from elementary perturbative arguments. One of the questions addressed in this work is to examine the potential impact of the center-of-mass contamination in truncated CI calculations on the results for ^{16}O, particularly when compared to other sources of errors that all approximate many-body methods using computationally tractable truncated model spaces carry.

For practical applications in nuclear structure calculations, the dimensions of the NCSM and CI model spaces become prohibitively large, even in relatively small systems, including the ^{16}O nucleus examined in this work, and even when we use the truncated CI approaches. For example, in the aforementioned CISDTQ $\equiv$ CI(4p4h) method one has to deal with huge numbers of $\sim n_o^3 n_u^3$ and $\sim n_o^4 n_u^4$ determinants of the 3p3h and 4p4h types and the iterative diagonalization steps that scale as $n_o^4 n_u^6$, where n_o and n_u are the numbers of occupied and unoccupied single-particle states, respectively. Therefore, in this study we introduce an additional physically motivated truncation of the CI and NCSM model spaces, which defines the importance-truncated (IT) CI and NCSM methods [39,63]. The IT-CI and IT-NCSM schemes are similar in the overall philosophy to the configuration selection techniques used in the quantum-chemical MRD-CI model of Peyerimhoff and Buenker [57,64,65]. Using the multiconfigurational perturbation theory of Ref. [66], we estimate the importance of individual basis states for the description of a certain target state. The amplitude with which a many-body basis state $|\Phi_\nu\rangle$ contributes in the first-order perturbation theory to an initial approximation $|\Psi_{\rm ref}\rangle$ of the target state of interest, e.g., the ground state $|\Psi_0\rangle$, defines an *a priori* importance measure

$$\kappa_\nu = -\frac{\langle\Phi_\nu|\, H_{\rm int}\,|\Psi_{\rm ref}\rangle}{\epsilon_\nu - \epsilon_{\rm ref}}, \tag{2}$$

where $\epsilon_\nu - \epsilon_{\rm ref}$ is the unperturbed excitation energy resulting from a Møller-Plesset-type partitioning of the Hamiltonian [66]. With the intrinsic Hamiltonian $H_{\rm int} = T - T_{\rm c.m.} + V_{\rm UCOM}$ being a two-body operator, the nonzero importance measures can be obtained only for the determinants $|\Phi_\nu\rangle$ that differ from the reference state $|\Psi_{\rm ref}\rangle$ by a 2p2h excitation at most.

To access higher-order mpmh excitations with $m > 2$, we embed the concept of the importance measure into an iterative construction of the importance-truncated model space. Starting from the lowest-energy Slater determinant $|\Phi_0\rangle$ as an initial reference $|\Psi_{\rm ref}\rangle$, all basis states with the importance measure $|\kappa_\nu| \geqslant \kappa_{\min}$, where $\kappa_{\min}$ defines the importance threshold, are included in the model space and the eigenvalue problem is solved. The resulting eigenvector, providing an improved approximation for the target state, is used to define the reference state $|\Psi_{\rm ref}\rangle$, which is now a multideterminantal state, for the second iteration and the above procedure is repeated. In the limit $\kappa_{\min} \to 0$, this iterative scheme converges to the full CI or NCSM space. The perturbative character of the importance measure entails an mpmh hierarchy. In the first iteration, only the determinants up to the 2p2h level are generated, resulting

in the IT-CI(2p2h) approximation. In the limit $\kappa_{\min} \to 0$, the IT-CI(2p2h) calculation recovers the full CISD $\equiv$ CI(2p2h) model space. In the second iteration, up to 4p4h determinants are present, leading to the CISDTQ $\equiv$ CI(4p4h) model space in the $\kappa_{\min} \to 0$ limit. In this study, we restrict ourselves to two iterations of IT-CI and IT-NCSM, i.e., model spaces up to the 4p4h level, so that the resulting IT-CI(4p4h) wave-function expansions are approximations to the CISDTQ wave functions. We should emphasize that for ^{16}O and for larger single-particle basis sets used in this study, the full CISDTQ $\equiv$ CI(4p4h) calculations would not be possible due to the prohibitively large dimensions of the corresponding model spaces. The IT methodology is among very few methods that enable one to incorporate 4p4h excitations in the CI calculations for nuclei with larger numbers of correlated particles, such as ^{16}O, and large single-particle basis sets with hundreds of orbitals in a computationally tractable fashion.

Eventually, as in the MRD-CI approach of Refs. [57,64,65], we construct the importance-truncated model spaces and solve the corresponding eigenvalue problems for a sequence of importance thresholds $\kappa_{\min}$ and extrapolate to $\kappa_{\min} \to 0$. All IT-NCSM and IT-CI results presented in Sec. IV are based on sequences of calculations with the importance thresholds in the range $\kappa_{\min} = 2 \times 10^{-5}$ to 15×10^{-5}. To warrant a robust extrapolation result, we use additional information from a second-order perturbative estimate for the energy contributions $\Delta_{\text{excl}}(\kappa_{\min})$ of the excluded determinants $|\Phi_\nu\rangle$, i.e., those determinants $|\Phi_\nu\rangle$ for which $|\kappa_\nu| < \kappa_{\min}$. In the limit of a vanishing threshold, which means that no determinants are discarded, we obviously have $\Delta_{\text{excl}}(0) = 0$. We employ this property as a constraint in a simultaneous extrapolation of the energies $E(\kappa_{\min})$ obtained from the truncated eigenvalue problem and of the perturbatively corrected energies $E(\kappa_{\min}) + \Delta_{\text{excl}}(\kappa_{\min})$ using fifth- to seventh-order polynomials for each of the quantities. The details of this procedure will be discussed elsewhere [63]. The uncertainties of the extrapolated energies reported in Sec. IV are always below 0.5 MeV.

The process of constructing the importance-truncated model spaces, combined with the extrapolation to the $\kappa_{\min} \to 0$ limit, as described above, is very efficient in reducing the dimensions of the corresponding CI or NCSM spaces to the many-body basis states that are most relevant for the eigenvalue problem of interest. Nevertheless, we still have to solve relatively large eigenvalue problems. Because the resulting eigenvalue problems involve sparse Hamiltonian matrices, we can use the Lanczos or Arnoldi technique to solve them. We use the ARPACK library for that purpose. The largest dimensions of the importance-truncated model spaces that appear in the calculations for ^{16}O presented in Sec. IV are a factor of a few times 10^7. Because we solve the eigenvalue problem in a restricted space, the importance-truncated CI and NCSM calculations fulfill the variational principle and the Hylleraas-Undheim theorem [67]. Furthermore, as in all CI and NCSM calculations, the IT-CI and IT-NCSM approaches provide us with easy access to the eigenstates of the Hamiltonian in a shell-model representation, along with the energies, without any additional effort. The IT-CI and IT-NCSM eigenstates can readily be used to compute expectation values of various observables, transition matrix elements, or densities and form factors.

If we stop the iterative construction of the importance-truncated model space before full self-consistency is reached, e.g., after just two iterations, as is done in this work, then the resulting IT-CI(4p4h) approach is not strictly size extensive. Thus, as in multireference CI calculations in quantum chemistry, where a similar problem occurs, we employ the aforementioned multireference Davidson (MRD) correction to estimate the effect of higher-order configurations beyond the 4p4h excitation level and to approximately restore size extensivity. We use the multireference rather than single-reference Davidson correction, because, in analogy to the multireference CI methods of quantum chemistry, the IT-CI(4p4h) wave function expansions contain subsets of the 3p3h and 4p4h determinants resulting from the up to 2p2h excitations from the multiconfigurational reference state $|\Psi_{\text{ref}}\rangle$. There are several ways of calculating the MRD extensivity corrections [57–61,68]. We use the Davidson-Silver form of the MRD correction discussed in Ref. [68], which we add to the IT-CI(4p4h) energy to obtain the final, approximately size extensive IT-CI(4p4h)+MRD result and which is calculated using the energy of the multiconfigurational reference state $|\Psi_{\text{ref}}\rangle$ and the summed weight of the reference determinants in the IT-CI(4p4h) eigenstate. By employing the *a posteriori* MRD corrections to IT-CI(4p4h) energies, we can incorporate the effects of the most essential higher-than-4p4h configurations in a computationally efficient manner without dealing with the higher-than-4p4h excitations explicitly. In the coupled-cluster methods discussed in Sec. III such contributions are represented by the disconnected product terms involving one- and two-body clusters. As shown in this work, the approximately size extensive IT-CI(4p4h)+MRD approach is competitive with the rigorously size extensive and accurate coupled-cluster schemes that are discussed in the following section.

III. COUPLED-CLUSTER METHOD

The second class of methods that we consider are those based on the single-reference coupled-cluster (CC) theory [69–73] (see Refs. [74–80] for selected reviews), which utilizes the exponential ansatz for the A-particle ground state,

$$|\Psi_0\rangle = \exp(T)|\Phi_0\rangle, \tag{3}$$

where $|\Phi_0\rangle$ is the reference determinant and

$$T = \sum_{k=1}^{A} T_k \tag{4}$$

is the cluster operator. The cluster operator T is a particle-hole excitation operator, defined relative to the Fermi vacuum $|\Phi_0\rangle$, whose many-body components

$$T_k = \sum_{i_1 < \cdots < i_k, a_1 < \cdots < a_k} t^{i_1 \ldots i_k}_{a_1 \ldots a_k} a^\dagger_{a_1} \cdots a^\dagger_{a_k} a_{i_k} \cdots a_{i_1} \tag{5}$$

generate the connected wave function diagrams of $|\Psi_0\rangle$ to infinite order. The remaining linked, but disconnected,

contributions are produced through the exponential ansatz for $|\Psi_0\rangle$. Here and elsewhere in this article, we use the notation in which $i_1, i_2, \ldots$ or $i, j, \ldots$ are the single-particle states occupied in the Fermi vacuum state $|\Phi_0\rangle$ and $a_1, a_2, \ldots$ or $a, b, \ldots$ are the single-particle states unoccupied in $|\Phi_0\rangle$ (we will use labels $p, q, \ldots$ for the generic single-particle basis states).

Typically, the explicit equations for the ground-state energy E_0 and the cluster amplitudes $t_{a_1\ldots a_k}^{i_1\ldots i_k}$ defining the many-body components T_k of T according to Eq. (5) are obtained by inserting the wave function $|\Psi_0\rangle$, Eq. (3), into the Schrödinger equation, $H|\Psi_0\rangle = E_0|\Psi_0\rangle$, premultiplying both sides of the resulting equation on the left by $\exp(-T)$ to obtain the connected cluster form of the Schrödinger equation [71,72],

$$\bar{H}|\Phi_0\rangle = E_0|\Phi_0\rangle, \tag{6}$$

where

$$\bar{H} = \exp(-T)H\exp(T) = [H\exp(T)]_C \tag{7}$$

is the similarity-transformed Hamiltonian or, equivalently, the connected product of the Hamiltonian and $\exp(T)$ (designated by subscript C), and projecting both sides of Eq. (6) on the reference determinant $|\Phi_0\rangle$ and excited determinants $|\Phi_{i_1\ldots i_k}^{a_1\ldots a_k}\rangle = a_{a_1}^\dagger \cdots a_{a_k}^\dagger a_{i_k}\cdots a_{i_1}|\Phi_0\rangle$ that span the relevant A-particle Hilbert space. The latter projections result in a nonlinear system of explicitly connected and energy-independent equations for the cluster amplitudes $t_{a_1\ldots a_k}^{i_1\ldots i_k}$,

$$\left\langle \Phi_{i_1\ldots i_k}^{a_1\ldots a_k}\right|\bar{H}|\Phi_0\rangle = 0, \quad i_1 < \cdots < i_k, \quad a_1 < \cdots < a_k, \tag{8}$$

where $\bar{H}$ is defined by Eq. (7) and $k = 1, \ldots, A$, whereas the projection on $|\Phi_0\rangle$ results in the CC energy formula,

$$E_0 = \langle\Phi_0|\bar{H}|\Phi_0\rangle. \tag{9}$$

The advantage of this formulation of CC theory, which is a standard formulation adopted, for example, in quantum chemistry, where most of the development and application work involving CC methods has occurred, is that, unlike the expectation value of the Hamiltonian with the CC wave function, which would lead to a nonterminating power series in T of the form $E_0 = \langle\Phi_0|[\exp(T^\dagger)H\exp(T)]_C|\Phi_0\rangle$ [72], the CC equations written above represent algebraic expressions that mathematically terminate at a finite power of T. The similarity-transformed Hamiltonian $\bar{H}$, or the connected product of the Hamiltonian and the $\exp(T)$ operator that is equivalent to $\bar{H}$ [cf. Eq. (7)], is a finite polynomial expansion in T whose length depends only on the highest many-body rank of the interactions in the Hamiltonian, not on the number of particles in a system, so one does not need to make *ad hoc* truncations in powers of T, which would have to be invoked if one attempted to minimize the expectation value of the Hamiltonian, to solve for the cluster amplitudes and energy. For example, for Hamiltonians that do not contain higher-than-pairwise interactions, $\bar{H}$ and the resulting CC equations for cluster amplitudes, Eq. (8), terminate at the T^4 terms, which is a purely mathematical truncation resulting from the fact that one cannot connect more than four T diagrams to the diagrams representing the Hamiltonian in the definition of $\bar{H}$, Eq. (7), if H is a two-body Hamiltonian. The energy formula, Eq. (9), simplifies even further in this case. If H does not contain higher-than-pairwise interactions, we obtain

$$E_0 = \langle\Phi_0|H|\Phi_0\rangle + \langle\Phi_0|\left[H_N\left(T_1 + T_2 + \tfrac{1}{2}T_1^2\right)\right]_C|\Phi_0\rangle, \tag{10}$$

where $H_N = H - \langle\Phi_0|H|\Phi_0\rangle$ is the Hamiltonian in the normal-ordered form relative to $|\Phi_0\rangle$. In other words, after determining the cluster operator T by solving the system of equations represented by Eq. (8), we only need the 1p1h or singly excited and 2p2h or doubly excited components of T, T_1, and T_2, respectively, to determine the energy if H is a two-body Hamiltonian.

The above is the exact CC theory, which is equivalent to the exact diagonalization of the Hamiltonian with the full CI approach. Indeed, we could obtain Eqs. (8) and (9) by directly projecting the Schrödinger equation for the exact CC wave function $|\Psi_0\rangle$, Eq. (3), $H\exp(T)|\Phi_0\rangle = E_0\exp(T)|\Phi_0\rangle$, with T defined by Eq. (4), on the $|\Phi_0\rangle$ and $|\Phi_{i_1\ldots i_k}^{a_1\ldots a_k}\rangle$ determinants that span the A-particle Hilbert space. The energy-dependent terms on the right-hand side of the resulting equations,

$$\left\langle \Phi_{i_1\ldots i_k}^{a_1\ldots a_k}\right|H\exp(T)|\Phi_0\rangle = E_0\left\langle \Phi_{i_1\ldots i_k}^{a_1\ldots a_k}\right|\exp(T)|\Phi_0\rangle, \tag{11}$$

cancel out the unlinked terms on the left-hand side of Eq. (11) to produce the system of the explicitly connected amplitude equations represented by Eq. (8) (see, e.g., Ref. [81] for a pedagogical derivation). Similarly, the disconnected diagrams corresponding to the product of the Hamiltonian and $\exp(T)$ in the resulting energy formula,

$$E_0 = \langle\Phi_0|H\exp(T)|\Phi_0\rangle, \tag{12}$$

do not contribute to Eq. (12), resulting in Eq. (9). Alternatively, one can show that Eq. (9) is equivalent to the expectation value of the Hamiltonian with the CC wave function, $\langle\Phi_0|\exp(T^\dagger)H\exp(T)|\Phi_0\rangle / \langle\Phi_0|\exp(T^\dagger)\exp(T)|\Phi_0\rangle$, as long as the cluster operator T has the exact form given by Eq. (4), in which all many-body components of T including T_A are included, and as long as the corresponding cluster amplitudes $t_{a_1\ldots a_k}^{i_1\ldots i_k}$ with $k = 1, \ldots, A$ satisfy Eq. (8) (see, e.g., Ref. [82]).

The exact CC theory, as described above, being equivalent to the full CI diagonalization, is limited to small few-body problems. Thus, in all practical applications of CC theory, including those reported in this work, one truncates the many-body expansion for T at some, preferably low, mpmh excitation level T_m. In this study, following the footsteps of quantum chemistry, where the CC theory has become one of the most successful and frequently used many-body methodologies, we focus on the most practical CC approximations that can be applied to systems with dozens or even hundreds of correlated fermions. Thus, we consider the basic CCSD (CC singles and doubles) approximation [83–86], which accounts for the effects of one- and two-body clusters, T_1 and T_2, respectively, as well as the completely renormalized CR-CC(2,3) approach [87–89], which accounts for the effects of connected three-body T_3 clusters through a relatively inexpensive, yet very effective, noniterative correction to the CCSD energy and which represents an improved variant of the completely renormalized CCSD(T) [CR-CCSD(T)] method [77,78,81,90] used in previous *ab initio* no core calculations for

the ^{4}He and ^{16}O nuclei [47–50]. In addition to many successful quantum chemistry applications (see Refs. [87–89,91–100] for representative examples), the CR-CC(2,3) approach was recently used to study the ground and excited states of the ^{56}Ni nucleus, treated by the effective Hamiltonian in the pf-shell basis [53], demonstrating its ability to provide a virtually exact description of closed-shell nuclei at a tiny fraction of the costs of the shell-model calculations that aim at similar accuracies, such as the CI method with up to 4p4h excitations, and the ability to retain the accuracy of the CI approach with up to 4p4h excitations even when the reference determinant contributes very little to the wave function [the CPU timings of the CR-CC(2,3) calculations reported in Ref. [53] were on the order of one minute on a single processor]. The present article shows the high accuracy offered by the CR-CC(2,3) approach in the context of the much larger scale no-core *ab initio* calculations for ^{16}O employing realistic nucleon-nucleon interactions and single-particle bases as large as eight major oscillator shells (480 uncoupled single-particle basis states).

In the CCSD calculations, which, in addition to producing reasonably accurate results for closed-shell systems, provide the framework for the determination of the CR-CC(2,3) corrections due to T_3 clusters, the many-body expansion of the cluster operator T defining the CC wave function ansatz is truncated at the level of 2p2h (or double) excitations, i.e., $T = T_1 + T_2$, where [cf. Eq. (5)]

$$T_1 = \sum_{i,a} t_a^i a_a^\dagger a_i \tag{13}$$

and

$$T_2 = \sum_{i<j,a<b} t_{ab}^{ij} a_a^\dagger a_b^\dagger a_j a_i \tag{14}$$

are the singly and doubly excited clusters. In analogy to the exact CC theory defined by Eqs. (8), where $k = 1, \ldots, A$, and (9), we determine the cluster amplitudes t_a^i and t_{ab}^{ij} defining the CCSD wave function

$$\left|\Psi_0^{(\mathrm{CCSD})}\right\rangle = \exp(T_1 + T_2)|\Phi_0\rangle \tag{15}$$

by solving the nonlinear system of energy-independent and explicitly connected algebraic equations similar to Eq. (8). Specifically, because we only need the T_1 and T_2 cluster components, we consider the subset of equations corresponding to the projections on the singly and doubly excited determinants [Eq. (8) with $k = 1$ and 2], so that the number of equations matches the number of unknown amplitudes t_a^i and t_{ab}^{ij}. We obtain

$$\left\langle \Phi_i^a \middle| \bar{H}^{(\mathrm{CCSD})} \middle| \Phi_0 \right\rangle = 0, \tag{16}$$

$$\left\langle \Phi_{ij}^{ab} \middle| \bar{H}^{(\mathrm{CCSD})} \middle| \Phi_0 \right\rangle = 0, \tag{17}$$

where

$$\begin{aligned} \bar{H}^{(\mathrm{CCSD})} &= \exp(-T_1 - T_2) H \exp(T_1 + T_2) \\ &= [H \exp(T_1 + T_2)]_C \end{aligned} \tag{18}$$

is the similarity-transformed Hamiltonian of CCSD [the similarity-transformed Hamiltonian $\bar{H}$, Eq. (7), written for $T = T_1 + T_2$], and $|\Phi_i^a\rangle$ and $|\Phi_{ij}^{ab}\rangle$ are the singly and doubly excited determinants, respectively, relative to $|\Phi_0\rangle$. Once the cluster amplitudes t_a^i and t_{ab}^{ij} defining T_1 and T_2 are known, the CCSD energy $E_0^{(\mathrm{CCSD})}$ is computed using Eq. (9) in which $\bar{H}$ is replaced by $\bar{H}^{(\mathrm{CCSD})}$, Eq. (18).

As pointed out above, the CC equations obtained through projections of the Schrödinger equation have finite polynomial nature, i.e., they terminate at a finite power of T that depends on the highest many-body rank of the interactions in the Hamiltonian. When the Hamiltonian is a two-body operator, the CC equations for cluster amplitudes terminate at the T^4 terms and the ground-state energy is given by Eq. (10). In particular, when H does not contain higher-than-two-body interactions, the generic CCSD amplitude equations, Eqs. (16) and (17), that apply to all Hamiltonians simplify to

$$\left\langle \Phi_i^a \middle| \left[H_N \left(1 + T_1 + T_2 + \tfrac{1}{2}T_1^2 + T_1 T_2 + \tfrac{1}{6}T_1^3\right)\right]_C \middle| \Phi_0 \right\rangle = 0 \tag{19}$$

and

$$\begin{aligned} \left\langle \Phi_{ij}^{ab} \middle| \left[H_N \left(1 + T_1 + T_2 + \tfrac{1}{2}T_1^2 + T_1 T_2 + \tfrac{1}{6}T_1^3 + \tfrac{1}{2}T_2^2 \right.\right.\right. \\ \left.\left.\left. + \tfrac{1}{2}T_1^2 T_2 + \tfrac{1}{24}T_1^4\right)\right]_C \middle| \Phi_0 \right\rangle = 0, \end{aligned} \tag{20}$$

respectively. If the cluster operator T was not truncated, as in the exact CC theory defined by Eqs. (4), (8), and (9), the results would be equivalent to the variational, full CI calculation corresponding to the minimization of the expectation value of the Hamiltonian with the CC wave function $|\Psi_0\rangle$, Eq. (3). Unfortunately, in the CCSD case, T is truncated at T_2, so that the resulting ground-state energy $E_0^{(\mathrm{CCSD})}$, determined by solving the CCSD amplitude equations, Eqs. (16) and (17) [or, when the Hamiltonian is two-body, Eqs. (19) and (20)], and by using the resulting T_1 and T_2 clusters in Eq. (9) [or, in the two-body Hamiltonian case, (10)] is not equivalent to the expectation value of the Hamiltonian with the CCSD wave function $|\Psi_0^{(\mathrm{CCSD})}\rangle$, Eq. (15), and, as such, does not have the bound if $A > 2$. One could, at least in principle, contemplate variational CCSD calculations based on minimizing the expectation value of the Hamiltonian with the CCSD wave function, as in Refs. [101,102], but, as already explained, the expectation value of the Hamiltonian with the CC (e.g., CCSD) wave function is a nonterminating series in cluster amplitudes that does not lead to practical computational schemes. On the other hand, due to the exponential nature of the CC wave function, the approximate CC methods using truncated cluster operators $T = \sum_{k=1}^{m} T_k$ with $m < A$ (CCSD corresponds to the $m = 2$ case) converge more rapidly to the full CI limit as $m \to A$ than the equivalent truncated shell-model expansions that rely on the same manifold of excited determinants, defined by Eq. (1), while providing the rigorously size extensive results that truncated CI expansions cannot provide due to the presence of unlinked contributions in the wave function and disconnected contributions in the energy that do not cancel out. For example, as already established in the 1970s and early 1980s, the CCSD method, which relies on up to 2p2h cluster components, is more accurate than the CI approach truncated at 2p2h determinants. As mentioned earlier, and as demonstrated in this article, the CCSD approach corrected for the connected 3p3h clusters T_3 via the CR-CC(2,3) method is as accurate as the CI approach with up to

4p4h excitations, while providing a size extensive description of many-particle systems. The issue of the lack of extensivity in CI calculations is addressed in this article through the suitably defined, quantum-chemistry-inspired corrections to the CI energies, as described in the previous section. The elementary analysis that enables one to understand why the CR-CC(2,3) method is as accurate as the CI approach with up to 4p4h excitations is provided in Sec. IV C.

The CCSD approximation provides information about the bulk of the correlation effects, which are described by T_1, T_2, and their products, but one must account for the higher-than-doubly excited connected clusters, particularly the T_3 clusters, to obtain a more quantitative description. This can be done through the CCSDT (CC singles, doubles, and triples) method [103,104], in which the cluster operator is truncated at the 3p3h level ($T = T_1 + T_2 + T_3$) and, in addition to the equations corresponding to the projections on singly and doubly excited determinants, one considers the projections on triply excited determinants [$k = 3$ in Eq. (8)]. Unfortunately, as explained below, the CCSDT scheme has very large computational costs, and so is generally not practical and limited to small few-body problems and relatively small single-particle basis sets. As a result, inspired by the similar difficulties encountered in quantum chemistry, where CCSDT is limited to small few-electron systems, we instead use the considerably less expensive CR-CC(2,3) approach, in which we incorporate the effects of T_3 clusters by adding a noniterative *a posteriori* correction

$$\delta_0(2,3) = \sum_{i<j<k,a<b<c} \ell_{ijk}^{abc} \mathfrak{M}_{abc}^{ijk} \tag{21}$$

to the CCSD energy $E_0^{(\mathrm{CCSD})}$ so the final CR-CC(2,3) energy is

$$E_0^{(\text{CR-CC(2,3)})} = E_0^{(\mathrm{CCSD})} + \delta_0(2,3), \tag{22}$$

where $\delta_0(2,3)$ is given by Eq. (21). The quantities $\mathfrak{M}_{abc}^{ijk}$ entering Eq. (21) are the projections of the connected cluster form of the Schrödinger equation written for the CCSD wave function on the triply excited determinants $|\Phi_{ijk}^{abc}\rangle$, which define the triply excited moments of the CCSD equations [77,78,81,87–90], i.e.,

$$\mathfrak{M}_{abc}^{ijk} = \langle \Phi_{ijk}^{abc} | \bar{H}^{(\mathrm{CCSD})} | \Phi_0 \rangle, \tag{23}$$

where $\bar{H}^{(\mathrm{CCSD})}$ is the similarity-transformed Hamiltonian of the CCSD approach, Eq. (18). As in the case of the CCSD equations, the explicit form of Eq. (23) depends on the nature of the interactions in the Hamiltonian. When the Hamiltonian does not contain higher–than–two-body interactions (the case examined in this article), one can write

$$\begin{aligned}\mathfrak{M}_{abc}^{ijk} = \langle \Phi_{ijk}^{abc} | \big[H_N \big(T_2 + T_1 T_2 + \tfrac{1}{2} T_2^2 + \tfrac{1}{2} T_1^2 T_2 \\ + \tfrac{1}{2} T_1 T_2^2 + \tfrac{1}{6} T_1^3 T_2 \big) \big]_C | \Phi_0 \rangle.\end{aligned} \tag{24}$$

The ℓ_{ijk}^{abc} coefficients entering Eq. (21) are defined as

$$\ell_{ijk}^{abc} = \langle \Phi_0 | \Lambda \bar{H} | \Phi_{ijk}^{abc} \rangle / D_{abc}^{ijk}, \tag{25}$$

where the denominator

$$D_{abc}^{ijk} = E_0^{(\mathrm{CCSD})} - \langle \Phi_{ijk}^{abc} | \bar{H}^{(\mathrm{CCSD})} | \Phi_{ijk}^{abc} \rangle \tag{26}$$

is obtained by approximating the triples-triples block of the matrix representing the $\bar{H}^{(\mathrm{CCSD})}$ operator, Eq. (18), by its diagonal, as in the Epstein-Nesbet perturbation theory, while $\Lambda = \Lambda_1 + \Lambda_2$ is the hole-particle de-excitation operator defining the CCSD "bra" or dual ground state [105–107]

$$\langle \tilde{\Psi}_0^{(\mathrm{CCSD})} | = \langle \Phi_0 | (1 + \Lambda_1 + \Lambda_2) \exp(-T_1 - T_2), \tag{27}$$

which satisfies the biorthonormality condition $\langle \tilde{\Psi}_0^{(\mathrm{CCSD})} | \Psi_0^{(\mathrm{CCSD})} \rangle = 1$. The one- and two-body components of the Λ operator of CCSD,

$$\Lambda_1 = \sum_{i,a} \lambda_i^a a_i^\dagger a_a \tag{28}$$

and

$$\Lambda_2 = \sum_{i<j,a<b} \lambda_{ij}^{ab} a_i^\dagger a_j^\dagger a_b a_a, \tag{29}$$

respectively, are obtained by solving the linear system of equations [105–107]

$$\langle \Phi_0 | (1 + \Lambda_1 + \Lambda_2) \bar{H}^{(\mathrm{CCSD})} | \Phi_i^a \rangle = E_0^{(\mathrm{CCSD})} \lambda_i^a, \tag{30}$$

$$\langle \Phi_0 | (1 + \Lambda_1 + \Lambda_2) \bar{H}^{(\mathrm{CCSD})} | \Phi_{ij}^{ab} \rangle = E_0^{(\mathrm{CCSD})} \lambda_{ij}^{ab}. \tag{31}$$

The details of the derivation of the noniterative correction $\delta_0(2,3)$ defining the CR-CC(2,3) calculations, which originates from the mathematical formalism referred to as the biorthogonal method of moments of coupled-cluster equations [87,88] and which describes the leading terms toward the full CI energy due to T_3 clusters, mimicking the performance of the much more expensive CCSDT method at the small fraction of the computer cost, can be found in Refs. [87,88].

The fact that the construction of the CR-CC(2,3) correction $\delta_0(2,3)$ requires the determination of the Λ operator of the CCSD theory, which defines the CCSD bra state $\langle \tilde{\Psi}_0^{(\mathrm{CCSD})} |$, as described above, has an additional advantage that we can use the same operator Λ to determine properties other than energy. We can, for example, use it to determine the CCSD one-body reduced density matrices

$$\begin{aligned}\gamma_q^p &\equiv \langle \tilde{\Psi}_0^{(\mathrm{CCSD})} | (a_p^\dagger a_q) | \Psi_0^{(\mathrm{CCSD})} \rangle \\ &= \langle \Phi_0 | (1 + \Lambda_1 + \Lambda_2) \overline{(a_p^\dagger a_q)} | \Phi_0 \rangle\end{aligned} \tag{32}$$

and properties

$$\langle \tilde{\Psi}_0^{(\mathrm{CCSD})} | \Theta | \Psi_0^{(\mathrm{CCSD})} \rangle = \sum_{p,q} \theta_p^q \gamma_q^p, \tag{33}$$

where Θ is a one-body property operator defined through matrix elements $\theta_p^q \equiv \langle p | \theta | q \rangle$,

$$\begin{aligned}\overline{(a_p^\dagger a_q)} &= \exp(-T_1 - T_2)(a_p^\dagger a_q) \exp(T_1 + T_2) \\ &= [(a_p^\dagger a_q) \exp(T_1 + T_2)]_C\end{aligned} \tag{34}$$

is the similarity-transformed connected form of the operator string $(a_p^\dagger a_q)$, analogous to the similarity-transformed Hamiltonian $\bar{H}^{(\mathrm{CCSD})}$, T_1 and T_2 are the singly and doubly excited clusters obtained by solving the CCSD equations, Eqs. (16) and (17), and Λ_1 and Λ_2 are obtained by solving the linear system of equations given by Eqs. (30) and (31) [105–107]. In general, if Ξ is an operator representing the quantum-mechanical

quantity of interest, the CC analog of the expectation value of Ξ can be determined using the equation [105–107]

$$\langle \Xi \rangle \equiv \langle \tilde{\Psi}_0 | \Xi | \Psi_0 \rangle = \langle \Phi_0 | (1 + \Lambda)\, \bar{\Xi} | \Phi_0 \rangle, \tag{35}$$

where

$$\bar{\Xi} = \exp(-T)\Xi \exp(T) = [\Xi \exp(T)]_C \tag{36}$$

is the similarity-transformed form of Ξ and Λ is the hole-particle de-excitation operator defining the left ground eigenstate of $\bar{H}$, Eq. (7), which has the form $\langle \Phi_0 | (1 + \Lambda)$, and the bra or dual CC ground state

$$\langle \tilde{\Psi}_0 | = \langle \Phi_0 | (1 + \Lambda) \exp(-T). \tag{37}$$

In analogy to the CCSD case, Λ can be obtained by solving the linear system of equations,

$$\langle \Phi_0 | (1 + \Lambda) \bar{H} \left| \Phi^{a_1 \ldots a_k}_{i_1 \ldots i_k} \right\rangle = E_0 \lambda^{a_1 \ldots a_k}_{i_1 \ldots i_k}, \tag{38}$$

where E_0 is the CC ground-state energy and $\lambda^{a_1 \ldots a_k}_{i_1 \ldots i_k}$ are the amplitudes that define the many-body components of Λ,

$$\Lambda_k = \sum_{i_1 < \cdots < i_k, a_1 < \cdots < a_k} \lambda^{a_1 \ldots a_k}_{i_1 \ldots i_k}\, a^\dagger_{i_1} \cdots a^\dagger_{i_k} a_{a_k} \cdots a_{a_1} \tag{39}$$

[clearly, Eq. (38) is the generalization of Eqs. (30) and (31), corresponding to the CCSD case, to any level of CC theory]. In particular, when Ξ is the Hamiltonian H, we obtain from Eq. (35)

$$\langle H \rangle = \langle \Phi_0 | (1 + \Lambda) \bar{H} | \Phi_0 \rangle, \tag{40}$$

which is equivalent to the CC energy formula, Eq. (9), since the $\langle \Phi_0 | \Lambda_k \bar{H} | \Phi_0 \rangle$ contributions to Eq. (40) vanish when the cluster operator T entering the definition of $\bar{H}$, as in Eq. (7), satisfies the system of CC equations, Eq. (8). It should be noted that the above way of calculating the $\langle \Xi \rangle$ values, which reflects on the biorthogonal character of CC theory, becomes fully equivalent to the determination of $\langle \Xi \rangle$ as the conventional expectation value $\langle \Psi_0 | \Xi | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle$ when T is a nontruncated cluster operator given by Eq. (4) obtained in the exact CC calculations defined by Eq. (8). When T is truncated, as in the CCSD case, the value of $\langle \Xi \rangle$ determined from Eq. (35), although no longer identical to the quantum-mechanical expectation value $\langle \Psi_0 | \Xi | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle$, where $|\Psi_0\rangle$ is the corresponding CC wave function, is equivalent to the alternative way of determining $\langle \Xi \rangle$ as $(\partial E_0(\lambda)/\partial \lambda)_{\lambda=0}$, where $E_0(\lambda)$ is the CC energy, Eq. (9), calculated after solving the relevant CC equations for the auxiliary Hamiltonian $H_\lambda = H + \lambda \Xi$, as in the response CC theory [82,108], as long as the reference determinant $|\Phi_0\rangle$ does not vary with λ. We use this fact in Sec. IV A to determine the expectation values of the center-of-mass Hamiltonian corresponding to the CCSD and CR-CC(2,3) calculations as the appropriate CC energy derivatives. The vast experience with performing CC calculations in quantum chemistry is that the difference between the values of $\langle \Xi \rangle$ calculated as the conventional quantum-mechanical expectation values and the $\langle \Xi \rangle$ values obtained as the corresponding energy derivatives, as described above, are very small, because the approximate CC methods, such as those used in this work, provide results close to full CI. Clearly, there are no differences between the $\langle \Xi \rangle$ values obtained as the traditional expectation values and energy derivatives in truncated CI calculations, because all CI methods are variational and, as such, satisfy the Hellmann-Feynman theorem. In approximate CC methods, we have to rely on a response formulation and the equations such as Eq. (35), or the equivalent energy derivatives, as described above, because, in analogy to the Hamiltonian, the traditional expectation value expression with the CC wave function, $\langle \Psi_0 | \Xi | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle$, would lead to a nonterminating power series in cluster amplitudes of the form $\langle \Phi_0 | [\exp(T^\dagger) \Xi \exp(T)]_C | \Phi_0 \rangle$ that does not lead to practical computational schemes.

By using the CR-CC(2,3) approach, we are able to significantly reduce the computational costs associated with the inclusion of the connected triply excited clusters, enabling calculations with relatively large model spaces, while producing results that should be as accurate as those obtained with the full CCSDT scheme [87]. Indeed, the most expensive computational steps of CR-CC(2,3) scale as $n_o^3 n_u^4$ in the determination of the noniterative correction due to T_3 and $n_o^2 n_u^4$ in the underlying CCSD calculation, where, as mentioned earlier, n_o and n_u represent the numbers of occupied and unoccupied single-particle states, respectively. For realistic values of n_o and n_u, including the larger single-particle basis sets used in this work, this is less expensive than the $n_o^3 n_u^5$ iterative steps defining CCSDT by orders of magnitude. In addition, unlike in CCSDT, in the CR-CC(2,3) calculations one does not have to store the large number of $\sim n_o^3 n_u^3$ amplitudes t^{ijk}_{abc} defining the T_3 cluster operator, because the noniterative correction $\delta_0(2, 3)$ defining the T_3 correction to the CCSD energy, Eq. (21), is calculated using the one- and two-body clusters, T_1 and T_2, and their Λ de-excitation analogs, Λ_1 and Λ_2, respectively, as described above, which need a storage of the $n_o n_u$ amplitudes t^i_a and λ^a_i and $n_o^2 n_u^2$ amplitudes t^{ij}_{ab} and λ^{ab}_{ij}. Thus, the total storage requirements of the CR-CC(2,3) calculations are primarily defined by the number of two-body matrix elements that define the Hamiltonian or the two-body matrix elements of the similarity-transformed Hamiltonian $\bar{H}^{(\mathrm{CCSD})}$. The memory requirements scale as $n_o n_u^3$. A small subset of the three-body matrix elements of $\bar{H}^{(\mathrm{CCSD})}$ that enter the calculation of the CR-CC(2,3) triples correction $\delta_0(2, 3)$ via the aforementioned equations for the Λ operator of CCSD and the triply excited moments $\mathfrak{M}^{ijk}_{abc}$ do not have to be precomputed and stored, because one can rigorously factorize the diagrams that represent them and express all quantities that enter the calculation of $\delta_0(2, 3)$ in terms of the one- and two-body matrix elements of $\bar{H}^{(\mathrm{CCSD})}$ (see, e.g., Ref. [109], and references therein). Thanks to the consistent use of the recursively generated intermediates, including one- and two-body matrix elements of $\bar{H}^{(\mathrm{CCSD})}$, and fast matrix multiplication routines [110], as is always done in the most efficient, modern implementations of CC methods in quantum chemistry, our CCSD and CR-CC(2,3) computer codes are fully vectorized. Thanks to the DIIS algorithm [111], which we use to solve the CCSD equations and their Λ counterparts (for the first application of the DIIS procedure to solving the CC equations, see Ref. [112]), our CCSD calculations typically converge in about 20 iterations to obtain an energy accurate to within 10^{-5} MeV. The triples correction $\delta_0(2, 3)$ requires no itera-

tions, which is one of the biggest advantages of CR-CC(2,3) as opposed to the iterative CCSDT approach. We refer the reader to Refs. [87–89] for the details of the CR-CC(2,3) theory, Ref. [109] for the explicit, computationally efficient expressions for the one- and two-body matrix elements of $\bar{H}^{(\mathrm{CCSD})}$ and moments $\mathfrak{M}^{ijk}_{abc}$ that enter the CR-CC(2,3) calculations, and Ref. [51] for the computationally efficient, fully factorized form of the CCSD equations that precede the calculation of the triples correction $\delta_0(2,3)$. We also note that although the earlier form of the CR-CC(2,3) approach, designated as CR-CCSD(T) [77,78,81,90], which was used in the studies of the ^{4}He and ^{16}O nuclei [47,48], was only approximately size extensive (to within 0.5–1% of the correlation energy [77]), the CR-CC(2,3) method used in this work is fully size extensive, so that no loss of accuracy occurs when going from smaller to larger many-fermion systems.

One of the most important findings of this work is that the CR-CC(2,3) method, with its relatively inexpensive computational steps that scale as $n_o^2 n_u^4$ in the iterative part and $n_o^3 n_u^4$ in the noniterative part, is capable of providing the results that are virtually identical to those that effectively correspond to the diagonalization of the Hamiltonian using the CI approach with up to 4p4h excitations from the reference determinant $|\Phi_0\rangle$, corrected for the effects of higher-than-4p4h excitations and extensivity through the use of the Davidson corrections. The IT-CI(4p4h) approach reduces the most expensive $n_o^4 n_u^6$ steps of the full CI(4p4h) calculation and the need to deal with the large numbers of the 3p3h and 4p4h determinants in the CI(4p4h) diagonalization by orders of magnitude through the use of importance truncation and extrapolation to the $\kappa_{\min} \to 0$ limit, as discussed in the previous section. The CR-CC(2,3) method does effectively the same work, eliminating, in particular, the need to deal with the 3p3h and 4p4h excitations of CI in an explicit manner, by representing the dominant higher-order correlations through the disconnected product terms involving low-order T_1 and T_2 clusters, such as, for example, $T_1 T_2$ for 3p3h excitations, $(1/2)T_2^2$ for 4p4h excitations, $(1/2)T_1 T_2^2$ for 5p5h excitations, $(1/6)T_2^3$ for 6p6h excitations, etc., while making sure that the connected 3p3h excitations that are usually more important than the disconnected $T_1 T_2$ terms are accounted for through the computationally affordable noniterative $\delta_0(2,3)$ correction to the CCSD energy. The detailed analysis of the CI and CC wave functions that explains this is provided in Sec. IV C. The numerical similarity of the CR-CC(2,3) and Davidson-corrected IT-CI(4p4h) [i.e., IT-CI(4p4h)+MRD)] results does not address the issue of the center-of-mass contaminations that are present in all truncated CC and all truncated CI calculations other than NCSM. The impact of the center-of-mass contaminations on the truncated CC [CCSD and CR-CC(2,3)] and CI [IT-CI(4p4h)] results for ^{16}O is examined in Sec. IV A.

IV. BENCHMARK FOR ^{16}O

We aim at a quantitative comparison of the different approaches using the ground state of ^{16}O as an example. For the interaction we use the realistic V_{UCOM} potential derived in the framework of the unitary correlation operator method (UCOM) discussed in Refs. [12–15]. Using a unitary transformation tailored for the description of short-range central and tensor correlations, a phase-shift equivalent soft interaction is derived from the Argonne V18 potential [1]. Applications in various many-body approaches, from the no-core shell model for light nuclei to Hartree-Fock and many-body perturbation theory for heavy nuclei [113], show that this two-body potential allows for a realistic description of binding energies throughout the nuclear chart without the explicit inclusion of additional three-body (or other higher-than-two-body) interactions. All calculations presented here are based on the same $V_{\mathrm{UCOM}}(I_\vartheta = 0.09\ \mathrm{fm}^3)$ potential as that used in Refs. [12,113].

As implied by the discussion in the previous section, we compare the following three groups of *ab initio* methods: (i) the coupled-cluster approach including singly and doubly excited clusters, CCSD, as well as the noniterative completely renormalized CR-CC(2,3) scheme that corrects the CCSD results for the effects of the connected triply excited clusters; (ii) the importance-truncated configuration interaction method including up to 4p4h excitations, IT-CI(4p4h), without and with the MRD size extensivity corrections; and (iii) the importance-truncated no-core shell model approach including up to 4p4h excitations, IT-NCSM(4p4h), with and without the MRD corrections. In addition to comparing the results of CC, CI, and NCSM calculations, particularly the CR-CC(2,3) and IT-CI(4p4h)(+MRD) levels, we examine several issues relevant for this comparison, including the role of center-of-mass contaminations and the sensitivity of the results to the choice of the single-particle basis. By comparing the size extensive, but not variationally bound CR-CC(2,3) results with the variational, but not rigorously size extensive IT-CI(4p4h)(+MRD) results for the binding energies of ^{16}O side by side, we have an opportunity to comment on the significance or insignificance of such issues as the violation of size extensivity by the truncated CI calculations and the lack of the variational bound in the CC calculations.

We begin with two important issues relevant for the comparison of the CCSD, CR-CC(2,3), IT-CI(4p4h)(+MRD), and IT-NCSM(4p4h) results, namely the role of center-of-mass contaminations and the sensitivity of the results to the choice of the single-particle basis.

A. Center-of-mass problem

All calculations are performed with a translationally invariant intrinsic Hamiltonian $H_{\mathrm{int}} = T - T_{\mathrm{c.m.}} + V_{\mathrm{UCOM}}$. However, this does not imply that the resulting many-body states and intrinsic energies are free of spurious contributions induced by a coupling of intrinsic and center-of-mass degrees of freedom. For the nucleus as a self-bound and translationally invariant system the intrinsic properties should not depend on the center-of-mass motion, i.e., intrinsic and center-of-mass components of the many-body state have to decouple.

For a Slater determinant basis, an exact separation of intrinsic and center-of-mass motions is possible only in a complete $N_{\max}\hbar\Omega$ model space based on harmonic oscillator

single-particle states as employed in the full NCSM approach. The use of a different model-space truncation or a different single-particle basis destroys this decoupling property and induces center-of-mass contaminations. This problem is well known in the context of the nuclear shell model (see Ref. [114] and references therein) and it was also addressed in the context of CC calculations for nuclei, both intrinsically, through a translationally invariant formulation [115,116], and numerically, through heuristic center-of-mass corrections added to the Hamiltonian [44–52].

To probe to what extent intrinsic and center-of-mass motions are coupled in the different many-body approaches examined in this work, we study the impact of an artificial shift of the center-of-mass spectrum using the Lawson prescription [114,117,118]. We introduce the modified Hamiltonian

$$H_\beta = H_{\rm int} + \beta H_{\rm c.m.}, \tag{41}$$

where

$$H_{\rm c.m.} = \frac{1}{2Am}\boldsymbol{P}^2_{\rm c.m.} + \frac{Am\Omega^2}{2}\boldsymbol{X}^2_{\rm c.m.} - \frac{3}{2}\hbar\Omega, \tag{42}$$

with center-of-mass momentum $\boldsymbol{P}_{\rm c.m.}$ and center-of-mass coordinate $\boldsymbol{X}_{\rm c.m.}$. If the center-of-mass motion is completely decoupled, then the expectation value of the intrinsic Hamiltonian $H_{\rm int}$, $\langle H_{\rm int}\rangle$, computed with the ground state resulting from the modified Hamiltonian H_β is independent of the value of β. Any dependence of $\langle H_{\rm int}\rangle$ on β indicates an unphysical coupling of intrinsic and center-of-mass motions and a violation of translational invariance.

In Table I we compare the results for the binding energy of ^{16}O obtained with the different many-body methods used in this work for two β values, namely $\beta = 0$, at which the initial intrinsic Hamiltonian is recovered, and $\beta = 10$, which is a typical empirical value used in shell-model applications [114]. We use the representative $\hbar\Omega$ values that approximately match the minima on the curves that describe the dependence of the relevant energies on $\hbar\Omega$. Because there is no rigorous criterion for choosing β, we will come back to the impact of variations of this parameter later on. The IT-CI(4p4h), IT-NCSM(4p4h), and NCSM values of $\langle H_{\rm int}\rangle$ and $\langle H_{\rm c.m.}\rangle$ are calculated directly as the standard quantum-mechanical expectation values of the relevant Hamiltonians using the eigenvectors obtained from the solution of the eigenvalue problem of H_β. The CCSD and CR-CC(2,3) analogs of $\langle H_{\rm int}\rangle$ at $\beta = 0$ are calculated using the appropriate CC energy formulas [Eq. (10) for CCSD and Eq. (22) for CR-CC(2,3)] applied to $H = H_{\rm int}$, rather than the expectation values of $H_{\rm int}$ with the CC wave functions that, as explained in Sec. III, are not used in the practical implementations of CC methods employed in this work. The CCSD and CR-CC(2,3) $\langle H_{\rm c.m.}\rangle$ values are obtained by numerically differentiating the corresponding energies, Eq. (10) for CCSD and Eq. (22) for CR-CC(2,3), where $H = H_\beta$, with respect to β at the β values of interest, as in the response CC considerations described in the previous section. Following the Lawson recipe, the CCSD and CR-CC(2,3) values of $\langle H_{\rm int}\rangle$ at nonzero β are calculated as $E_0(\beta) - \beta\langle H_{\rm c.m.}\rangle_\beta$, where $E_0(\beta)$ is the relevant CC [CCSD or CR-CC(2,3)] energy obtained for the center-of-mass-corrected Hamiltonian H_β and $\langle H_{\rm c.m.}\rangle_\beta = \partial E_0(\beta)/\partial\beta$ is the corresponding value of $\langle H_{\rm c.m.}\rangle$ calculated at the same β through the numerical differentiation of $E_0(\beta)$, as described above.

As Table I shows, the full NCSM approach allows an exact separation of intrinsic and center-of-mass motions and consequently the intrinsic energy $\langle H_{\rm int}\rangle$ is independent of β. The IT-NCSM(4p4h) method shows a minimal variation of the intrinsic energy at the level of 0.1 MeV, which is a consequence of the importance truncation. This tiny coupling in the IT-NCSM(4p4h) calculations can safely be neglected. The CCSD, CR-CC(2,3), and IT-CI(4p4h) methods violate translational invariance from the beginning through the choice of the model space. This results in a more sizable coupling between intrinsic and center-of-mass motions when compared to the IT-NCSM(4p4h) scheme: the intrinsic energies $\langle H_{\rm int}\rangle$ change by 2 to 3 MeV when going from $\beta = 0$ to $\beta = 10$. As mentioned above, the oscillator frequencies used in Table I correspond to the approximate positions of the minima on the curves that show the dependencies of the relevant energies on $\hbar\Omega$. The full $\hbar\Omega$ dependence of the intrinsic energies $\langle H_{\rm int}\rangle$ for $\beta = 0$ and $\beta = 10$ obtained in the CCSD and CR-CC(2,3) calculations is depicted in Fig. 1. Evidently, the change of $\langle H_{\rm int}\rangle$, when going from $\beta = 0$ to $\beta = 10$,

TABLE I. The CI and NCSM expectation values of $H_{\rm int}$ and $H_{\rm c.m.}$, and their CC analogs defined in the text (in units of MeV), obtained from the many-body solutions using H_β for $\beta = 0$ and $\beta = 10$. The CC and IT-CI calculations use a harmonic oscillator basis with $e_{\rm max} = 5$ and $\hbar\Omega = 30$ MeV, whereas the IT-NCSM and NCSM calculations use a model space with $N_{\rm max} = 8$ and $\hbar\Omega = 22$ MeV. The oscillator frequencies correspond to the respective energy minima of the CC and NCSM calculations.

	$\beta = 0$		$\beta = 10$	
	$\langle H_{\rm int}\rangle$	$\langle H_{\rm c.m.}\rangle$	$\langle H_{\rm int}\rangle$	$\langle H_{\rm c.m.}\rangle$
CCSD	−107.32	5.88	−104.84	0.24
CR-CC(2,3)	−113.14	5.38	−111.23	0.20
IT-CI(4p4h)	−98.67	1.37	−97.32	0.19
IT-NCSM(4p4h)	−104.10	0.08	−104.01	0.02
NCSM	−104.75	0.00	−104.75	0.00

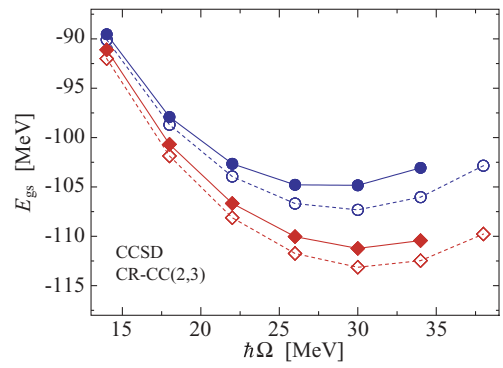

FIG. 1. (Color online) The intrinsic ground-state energies, $\langle H_{\rm int}\rangle$, of ^{16}O, obtained with the CCSD and CR-CC(2,3) approaches at $\beta = 0$ (open symbols) and $\beta = 10$ (filled symbols), as functions of $\hbar\Omega$ for a harmonic oscillator basis with $e_{\rm max} = 5$: CCSD (●, ○) and CR-CC(2,3) (♦, ◊).

increases somewhat with increasing oscillator frequency. For example, for $\hbar\Omega = 18$ MeV, the intrinsic energy obtained with the CR-CC(2,3) approach changes by 1.18 MeV when going from $\beta = 0$ to $\beta = 10$, whereas the analogous change in the CR-CC(2,3) energy for $\hbar\Omega = 34$ MeV is 2.03 MeV.

The above results demonstrate that the Lawson prescription is quite efficient in reducing the expectation value of the center-of-mass Hamiltonian, $\langle H_{\text{c.m.}} \rangle$, obtained from the CCSD, CR-CC(2,3), and IT-CI(4p4h) solutions, as shown in Table I. However, this does not mean that a decoupling between intrinsic and center-of-mass motions or a spuriousness-free intrinsic state has been completely achieved. In fact, if we take the same Lawson prescription and compare the intrinsic energies $\langle H_{\text{int}} \rangle$ for $\beta = 10$ and $\beta = 20$, we observe changes in the values of $\langle H_{\text{int}} \rangle$ that are similar in magnitude to those observed when one goes from $\beta = 0$ to $\beta = 10$. For example, for the IT-CI(4p4h) calculations at $\hbar\Omega = 30$ MeV using six major oscillator shells (i.e., $e_{\max} = 5$), the change in the $\langle H_{\text{int}} \rangle$ value when going from $\beta = 0$ to $\beta = 10$ is 1.35 MeV. When going from $\beta = 10$ to $\beta = 20$, the IT-CI(4p4h) value of the $\langle H_{\text{int}} \rangle$ energy changes by 0.91 MeV although $\langle H_{\text{c.m.}} \rangle$ at $\beta = 10$ is already below 0.2 MeV. This shows that the smallness of $\langle H_{\text{c.m.}} \rangle$ alone does not indicate a decoupling or warrant an intrinsic state free of center-of-mass contaminations.

Apart from an explicit projection [114] or a translationally invariant formulation, there is no rigorous way to eliminate the center-of-mass contamination problem from the CC and CI calculations. Of the methods presented in this work, only the NCSM and IT-NCSM calculations are free (in the IT-NCSM case, virtually free) of this spuriousness. The CC and CI results are center-of-mass contaminated although, as shown in Table I and Fig. 1, the degree of this contamination, when the harmonic oscillator reference $|\Phi_0\rangle$ is used, seems relatively small in the case of ^{16}O. Indeed, the degree of center-of-mass contamination, as measured by the changes in the intrinsic energies $\langle H_{\text{int}} \rangle$ when going from $\beta = 0$ to $\beta = 10$, does not seem to exceed 2–3 MeV when a medium-size single-particle basis consisting of six major oscillator shells is employed and $|\Phi_0\rangle$ is the harmonic oscillator reference, although we must remember that similar changes in the intrinsic energies are observed when going from $\beta = 10$ to $\beta = 20$, suggesting that the real degree of center-of-mass contamination in the CC and CI results is somewhat bigger than 2–3 MeV. The degree of center-of-mass contamination, as measured by the $\langle H_{\text{c.m.}} \rangle$ values at $\beta = 0$, does not seem to exceed about 5–6 MeV in the same basis. When the size of the single-particle basis is increased, as is done in the following sections where we examine single-particle basis sets as large as $e_{\max} = 7$ (eight major oscillator shells), the magnitude of the unphysical coupling of intrinsic and center-of-mass motions in the CC and CI calculations is expected to be reduced, since we approach the limit of the complete single-particle basis. On the other hand, other effects, such as the $\hbar\Omega$ dependencies of the resulting energies shown in Fig. 1 and the fact that the CCSD, CR-CC(2,3), and IT-CI(4p4h) methods do not provide the exact wave function that would factorize into the intrinsic and translational components, might hinder the reduction of the center-of-mass contaminations present in the CC and CI results. For all these various reasons, in the assessment of the quality of the CC and CI calculations reported in this work, we will remain cautious and keep in mind that the resulting ground-state energies may carry an uncertainty anywhere between 2 and 6 MeV or so as a result of center-of-mass contamination, at least when the harmonic oscillator reference $|\Phi_0\rangle$ is employed. We will continue examining the role of center-of-mass contaminations on the CCSD, CR-CC(2,3), and IT-CI(4p4h) calculations with different types of single-particle bases and different basis set sizes in the future work.

B. Role of the single-particle basis

In many cases, the harmonic oscillator basis is not the optimal choice for the expansion of the nuclear many-body state. The naive reference determinant $|\Phi_0\rangle$ obtained by occupying the lowest-energy harmonic oscillator states may have a relatively small overlap with the final wave function $|\Psi_0\rangle$, resulting in unnecessarily long CI expansions to represent the correlated $|\Psi_0\rangle$ state that have to compensate for the deficiencies of the reference determinant $|\Phi_0\rangle$. By switching to a single-particle basis optimized for the nucleus under consideration, generated, for example, by a Hartree-Fock calculation, the convergence with respect to the many-particle basis can be significantly enhanced. Generally, this option is not used in the NCSM calculations, because the use of a single-particle basis set other than the harmonic oscillator basis would destroy the mathematical decoupling of intrinsic and center-of-mass motions that the NCSM model space guarantees for any finite basis set. However, for the truncated CC or CI approaches, where we do not have this property anyway, we may benefit from the use of optimized single-particle bases.

To demonstrate the effect of an optimization of the single-particle basis, we compare the results of the CC and CI calculations using the harmonic oscillator (HO) and Hartree-Fock (HF) bases. The latter is obtained from a self-consistent Hartree-Fock calculation using the same intrinsic Hamiltonian H_{int} and the same single-particle space as those employed in the subsequent many-body calculations [113]. Therefore, the HF optimization can be viewed as a unitary transformation within the set of single-particle states employed in the many-body calculations. For a full CI calculation at given $e_{\max}$, where all determinants resulting from a given single-particle basis set are included, this transformation would not affect the results. The situation changes when one uses the truncated CI and CC wave function expansions, where the HO $\rightarrow$ HF transformation of single-particle states may have an effect on the resulting energies. As elaborated on below, this effect is expected to be small in the case of CC calculations, which rely on the exponential form of the wave function that makes the results of truncated CC calculations virtually invariant with respect to orbital rotations through the presence of the $\exp(T_1)$ component in the CC wave operator, as in the Thouless theorem [119], but can be quite significant when the truncated CI expansions are employed, because the CI wave operator is a linear rather than an exponential excitation operator that does not contain sufficiently many terms to make the results numerically invariant with respect to orbital rotations if

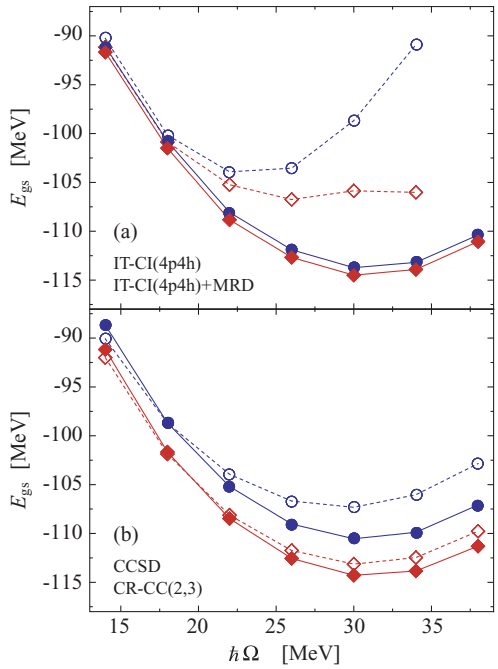

FIG. 2. (Color online) Ground-state energy of ^{16}O as a function of $\hbar\Omega$ obtained with the HO single-particle basis (open symbols) and the HF-optimized basis (filled symbols) in an $e_{\max} = 5$ model space. (a) Importance-truncated configuration interaction calculations: IT-CI(4p4h) (●, ○) and IT-CI(4p4h)+MRD (◆, ◇). (b) coupled-cluster calculations: CCSD (●, ○) and CR-CC(2,3) (◆, ◇).

truncated at the mpmh excitations with $m \ll A$. Our numerical analysis confirms these expectations.

The impact of the basis optimization on a IT-CI(4p4h) calculation is illustrated in Fig. 2(a), where we compare the HO- and HF-based IT-CI(4p4h) results obtained with the $e_{\max} = 5$ model space. We performed similar calculations using other model spaces up to and including $e_{\max} = 7$, and the results are very similar to those shown in Fig. 2(a), so in the following discussion we focus on the $e_{\max} = 5$ case. At smaller oscillator frequencies, the ground-state energies of ^{16}O obtained with both bases agree very well. However, with increasing $\hbar\Omega$ the HF basis leads to lower ground-state energies than the HO basis. At the same time, the Davidson correction for the HO-based calculation increases rapidly, indicating that contributions beyond the 4p4h level become significant in this case. In contrast to the HO-based IT-CI(4p4h) calculation, the HF-based IT-CI(4p4h) calculation develops a minimum at larger $\hbar\Omega$ and the Davidson correction remains small at all frequencies, clearly implying that the role of higher-than-4p4h excitations in the CI expansion of the ground-state wave function of ^{16}O is suppressed when the optimum HF determinant is used as a reference determinant $|\Phi_0\rangle$.

The analogous analysis for the CCSD and CR-CC(2,3) calculations, presented in Fig. 2(b), reveals that the CC methods are significantly less sensitive to the choice of the single-particle basis. Again, we show only the sample of the HO- and HF-based CCSD and CR-CC(2,3) calculations corresponding to the $e_{\max} = 5$ model space. We performed similar CC calculations using other model spaces up to and including $e_{\max} = 7$, and the observed patterns are similar to those shown in Fig. 2(b), so we focus on the $e_{\max} = 5$ case here. As was the case for the IT-CI(4p4h) calculations, the energies obtained with the two bases are virtually the same for smaller $\hbar\Omega$ values. As we increase the oscillator frequency, the disagreement between the HO- and HF-based CC results grows, but only slightly, particularly for the CR-CC(2,3) approach. Indeed, unlike the IT-CI(4p4h) case, where the largest discrepancies between the results obtained with the two bases in the $\hbar\Omega = 14$–34 MeV region, which occur at $\hbar\Omega = 34$ MeV, are as much as 8 MeV with the Davidson correction and about 20 MeV without it, the analogous differences between the HO- and HF-based CC results at larger $\hbar\Omega$ values are quite small, with the two results differing by 3.8(4.2) MeV in the CCSD case and 1.4(1.5) MeV in the CR-CC(2,3) case, when the $e_{\max} = 5$ basis set is employed and $\hbar\Omega = 34(38)$ MeV. Furthermore, we see that the overall shapes of the curves displaying the $\hbar\Omega$ dependence of the total energies obtained with the CCSD and CR-CC(2,3) approaches are very similar regardless of which single-particle basis is used. It is interesting to note that for both the CC and CI methodologies, the agreement between the results obtained with the two bases improves as we use more accurate approximations. This is particularly true for the CC calculations, where the difference between the HO- and HF-based results obtained with the CR-CC(2,3) method, which is a more accurate approximation when compared to CCSD, is smaller than the analogous difference between the HO- and HF-based CCSD results. The differences between the CI results obtained with the two bases are generally larger, but even in this case, the difference between the HO- and HF-based results obtained with the IT-CI(4p4h)+MRD approach, which corrects the IT-CI(4p4h) energies for at least some effects of higher-than-4p4h excitations, are smaller than the analogous difference between the HO- and HF-based IT-CI(4p4h) results. This makes sense, of course, because the closer we get to the full CI limit, the less sensitive the results become with respect to orbital rotations.

The relative insensitivity of the CC results to the choice of the single-particle basis, which has been known in quantum chemistry for a long time (cf., e.g., Ref. [120]), is a consequence of the implicit inclusion of the Thouless theorem [119] in the CC calculations through the $\exp(T_1)$ component of the CC wave operator $\exp(T)$, even when T is truncated at the two-body level, as in CCSD, where $T = T_1 + T_2$. The $\exp(T_1)$ component of the CCSD wave operator $\exp(T_1 + T_2) = \exp(T_1)\exp(T_2)$ (T_1 and T_2 are particle-hole excitation operators and hence they commute), obtained by solving the coupled system of equations for the T_1 and T_2 clusters, as described in Sec. III, acting on the reference determinant $|\Phi_0\rangle$ effectively optimizes the single-particle basis for the many-particle state of interest without the need for the explicit introduction of orbital relaxation, thus reducing the impact of any inadequacies of the basis on the final results and making the CCSD energies almost independent of the type of the single-particle basis. One can simply write the CCSD wave function, Eq. (15), as $|\Psi_0^{(\mathrm{CCSD})}\rangle = \exp(T_1 + T_2)|\Phi_0\rangle = \exp(T_2)|\Phi_0'\rangle$, where $|\Phi_0'\rangle = \exp(T_1)|\Phi_0\rangle$ is a new reference determinant

optimized for the ground-state $|\Psi_0^{(\mathrm{CCSD})}\rangle$ through the suitable choice of T_1 obtained from the CCSD calculations. Indeed, if we analyze the T_1 cluster amplitudes resulting from our CCSD calculations, we see that they are quite large when the HO basis and large $\hbar\Omega$ are employed, i.e., when the HO reference determinant $|\Phi_0\rangle$ is far from the optimum reference. When the optimized HF basis is employed, the T_1 cluster amplitudes resulting from CCSD calculations are small, independent of $\hbar\Omega$. These patterns are reflected in the values of the so-called T_1 Diagnostic [121], which is defined as $(\langle\Phi_0|T_1^\dagger T_1|\Phi_0\rangle/n_o)^{1/2}$. In defining the T_1 Diagnostic, we divide the connected (i.e., size extensive) quantity $\langle\Phi_0|T_1^\dagger T_1|\Phi_0\rangle$, which represents the magnitude of T_1 cluster contributions to the wave function, by n_o to make the result independent of the system size. For the case of the $e_{\max} = 5$ model space and the HO basis, the T_1 Diagnostic resulting from the CCSD calculations changes quite dramatically, from 0.10 at $\hbar\Omega = 14$ MeV to 0.42 at $\hbar\Omega = 38$ MeV and 0.48 at $\hbar\Omega = 42$ MeV, indicating a steep increase in the values of the T_1 cluster amplitudes due to the increasing inadequacy of the HO reference determinant $|\Phi_0\rangle$ at larger $\hbar\Omega$ values that those large T_1 amplitudes compensate for. For the optimized HF basis, the same diagnostic remains almost constant, with values that do not exceed 0.04 in the entire $\hbar\Omega = 14$–42 MeV region, confirming the smallness of T_1 cluster amplitudes independent of $\hbar\Omega$ in the HF-basis case. In fact, it is easy to understand why T_1 is small in the HF basis. When $|\Phi_0\rangle$ is the HF reference, the lowest orders of many-body perturbation theory that the T_1 cluster component contributes to are second for the wave function and fourth for the energy. For comparison, T_1 contributes to the first-order wave function and second-order correction to the energy when the non-HF references, such as the HO reference determinant, are used. In the region of larger $\hbar\Omega$ values, the HO reference determinant is so far from the optimum HF determinant that the resulting T_1 amplitudes become very large, as reflected in the above values of the T_1 Diagnostic.

To confirm that the primary role of the T_1 operator in CC calculations is to effectively relax the orbitals to produce the optimum reference determinant $|\Phi_0'\rangle = \exp(T_1)|\Phi_0\rangle$ for the many-particle state of interest, we compare the T_2 cluster operators resulting from the HO- and HF-based CCSD calculations. We expect the T_2 clusters, which describe the leading correlation effects, to be very similar in the HO- and HF-based CCSD calculations if the main role of T_1 is to optimize the reference determinant. The T_2 Diagnostic (cf., e.g., Ref. [53]), which is defined as $(\langle\Phi_0|T_2^\dagger T_2|\Phi_0\rangle/n_o)^{1/2}$ and which measures the significance of the T_2 cluster contributions, confirms this expectation. For the $e_{\max} = 5$ model space, the values of the T_2 Diagnostic obtained from the HO-based CCSD calculations are 0.17–0.18 in the entire $\hbar\Omega = 14$–42 MeV region. The analogous values of the T_2 Diagnostic resulting from the HF-based CCSD calculations are 0.15–0.17 in the same region. Thus, the T_2 clusters that describe the true correlation effects barely change with the type of the basis (HO vs. HF) and $\hbar\Omega$. The T_1 clusters remain small and do not change much with $\hbar\Omega$ when the optimized HF basis is employed, while becoming sizable in the large $\hbar\Omega$ region when the naive reference determinant $|\Phi_0\rangle$, obtained by filling the lowest-energy HO single-particle states, which is a poor representation of the correlated ground state in that region, is employed. The CC theory can cope with the inadequacy of the HO basis by using the $\exp(T_1)$ component of the CC wave operator with large T_1 amplitudes to transform the naive reference determinant $|\Phi_0\rangle$ resulting from the use of the HO basis, as in the Thouless theorem, to the more optimal form that is adjusted to the ground-state wave function $|\Psi_0\rangle$. The same $\exp(T_1)$ operator does not change the reference determinant $|\Phi_0\rangle$ too much when T_1 is small, i.e., when the orbitals are properly optimized beforehand, as in the HF case. This explains the virtual invariance of the CC results on the choice of the single-particle basis.

The same arguments enable us to understand why the results of truncated CI calculations may significantly depend on the type of the basis in the region of larger $\hbar\Omega$ values and why one needs to use the HF-optimized orbitals in that region to obtain the results of the CC quality with the truncated CI approaches. Let us focus on the IT-CI(4p4h) approach and the related CISDTQ scheme, in which the linear excitation operator C defining the ground-state wave function $|\Psi_0\rangle$ through the formula $|\Psi_0\rangle = C|\Phi_0\rangle$ has the truncated form $C = C_0 + C_1 + C_2 + C_3 + C_4$. Here, C_k is the $kpkh$ excitation operator generating the contributions from the k-tuply excited determinants when acting on $|\Phi_0\rangle$ (C_0 generates the reference contribution). When the intermediate normalization condition $\langle\Phi_0|\Psi_0\rangle = 1$ is imposed on the CI wave function, so that C_0 becomes a unit operator, the 1p1h component of the CI wave function, $C_1|\Phi_0\rangle$, is equivalent to the 1p1h component of the CC wave function, $T_1|\Phi_0\rangle$. In addition to the connected $T_1|\Phi_0\rangle$ contribution, the IT-CI(4p4h) and CISDTQ wave functions contain the disconnected cluster terms, such as $(1/2)T_1^2|\Phi_0\rangle$ (through the C_2 contribution), $(1/6)T_1^3|\Phi_0\rangle$ (through the C_3 contribution), and $(1/24)T_1^4|\Phi_0\rangle$ (through the C_4 contribution), but they do not contain the entire $\exp(T_1)|\Phi_0\rangle$ expansion, which includes higher powers of T_1 if $A > 4$ (as is the case for the ^{16}O nucleus). In other words, the linear excitation operators C of the IT-CI(4p4h) and CISDTQ approaches or other truncated CI schemes do not have the mathematical structure of the Thouless theorem that would enable one to factor out the $\exp(T_1)$ component that would make the results virtually independent of the orbital choice. In consequence, the results of truncated CI calculations may display a strong dependence on the choice of the basis, as our IT-CI(4p4h) calculations shown in Fig. 2 clearly demonstrate. Full CI is the only CI method that contains the $\exp(T_1)|\Phi_0\rangle$ component in its entirety, since one can always represent the intermediately normalized full CI wave function for the A-body system, $|\Psi_0\rangle = (1 + C_1 + \cdots + C_A)|\Phi_0\rangle$, in the exponential form $|\Psi_0\rangle = \exp(T_1 + \cdots + T_A)|\Phi_0\rangle$.

The analogous analysis can be used to explain why the HO-based IT-CI(4p4h) calculations become less accurate in the region of larger $\hbar\Omega$ values and why the IT-CI(4p4h) calculations benefit from the use of the HF-optimized orbitals, particularly in the region of larger $\hbar\Omega$ values. As already pointed out, the T_1 cluster component becomes large in the region of larger $\hbar\Omega$ values when the HO reference $|\Phi_0\rangle$ is employed. This can be seen by analyzing the CCSD wave function, as described above, or by examining the IT-CI(4p4h)

wave function. Because the 1p1h component of the CI wave function, $C_1|\Phi_0\rangle$, is equivalent to the 1p1h component of the CC wave function, $T_1|\Phi_0\rangle$, when the intermediate normalization is imposed, we can immediately conclude that if T_1 is large, as is the case for larger $\hbar\Omega$ values and HO basis, the corresponding C_1 excitation amplitudes should be large as well. This is exactly what we observe in the HO-based IT-CI(4p4h) calculations. For example, the largest C_1 excitation amplitude in the IT-CI(4p4h) intermediately normalized wave function increases from 0.08 at $\hbar\Omega =$ 14 MeV to 0.29 at $\hbar\Omega = 30$ MeV and 0.40 at $\hbar\Omega = 38$ MeV when the HO basis is used and $e_{\max} = 5$. In contrast, the HF-based IT-CI(4p4h) calculations exhibit largest C_1 amplitudes that do not exceed 0.03 throughout the entire $\hbar\Omega$ range. Now, if the C_1 or T_1 component is large, the product terms such as T_1T_2, $(1/2)T_1^2T_2$, $(1/6)T_1^3T_2$, $(1/2)T_1T_2^2$, $(1/4)T_1^2T_2^2$, etc., become relatively large as well. All of these terms are included in the CCSD wave function, helping the accuracy of the CCSD and CR-CC(2,3) calculations, but not all of them are present in the IT-CI(4p4h) wave function, which contains the T_1T_2 and $(1/2)T_1^2T_2$ components through the 3p3h and 4p4h contributions described by C_3 and C_4, respectively, but not the $(1/6)T_1^3T_2$, $(1/2)T_1T_2^2$, and $(1/4)T_1^2T_2^2$ components, which represent the 5p5h $[(1/6)T_1^3T_2$ and $(1/2)T_1T_2^2]$ and 6p6h $[(1/4)T_1^2T_2^2]$ excitations neglected in IT-CI(4p4h). As we can see, the absence of the 5p5h, 6p6h, etc., components in the IT-CI(4p4h) wave function hurts the accuracy of the IT-CI(4p4h) calculations when C_1 or T_1 is large, which is exactly what happens when we use the HO basis in the region of larger $\hbar\Omega$ values.

The situation dramatically changes when the HF basis is employed. In that case, the C_1 or T_1 contributions are small and the higher-order product terms, such as $(1/6)T_1^3T_2$, $(1/2)T_1T_2^2$, and $(1/4)T_1^2T_2^2$, which are neglected in the IT-CI(4p4h) calculations, become very small as well, resulting in an excellent description of the ^{16}O nucleus by the IT-CI(4p4h) method in the entire region of $\hbar\Omega$ that matches the accuracy of the CR-CC(2,3) calculations, particularly when the already very good IT-CI(4p4h) results are corrected for size extensivity and the remaining small higher-than-4p4h excitations through the multireference Davidson correction. The excellent agreement between the HF-based IT-CI(4p4h)+MRD and CR-CC(2,3) results, illustrated in Fig. 2 for $e_{\max} = 5$, remains valid when larger model spaces are employed, enabling us to draw several important conclusions regarding the quality of the *ab initio* results for ^{16}O reported in this work. These conclusions are discussed in the next section.

C. Comparison of large-scale calculations

We now compare the predictions for the ground-state energy of ^{16}O obtained in the IT-NCSM, IT-CI, and CC calculations employing V_{UCOM} and the largest model spaces that we could handle with a reasonable computational effort.

In Fig. 3 the convergence of the IT-NCSM ground-state energy as a function of $N_{\max}$ is shown for fixed $\hbar\Omega =$ 22 MeV, which is determined by the position of the energy minimum for the larger model spaces [63]. In addition to

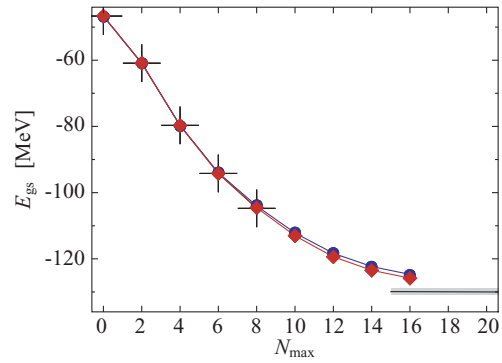

FIG. 3. (Color online) Importance-truncated no-core shell-model calculations for the ground-state energy of ^{16}O with V_{UCOM} for $\hbar\Omega = 22$ MeV. Shown are the results of the IT-NCSM(4p4h) calculations (●), IT-NCSM(4p4h)+MRD calculations (⧫), and full NCSM calculations (+). The vertical line indicates the result of an exponential extrapolation of the IT-NCSM(4p4h)+MRD energies.

the IT-NCSM(4p4h) results without and with the Davidson correction, we report the results of full NCSM calculations using the ANTOINE code [122] for $N_{\max} \leqslant 8$. In the region where these exact reference results are available, the IT-NCSM(4p4h)+MRD and full NCSM energies agree to within 0.1 MeV or better.

Using exponential fits involving the five largest model spaces [123], we obtain an extrapolated ground-state energy of (-129 ± 1) MeV for the IT-NCSM(4p4h) data and of (-130 ± 1) MeV for the IT-NCSM(4p4h)+MRD results. The change due to the Davidson correction provides an estimate of the effects beyond 4p4h configurations. This estimate agrees very well with the preliminary results of the explicit inclusion of up to 6p6h configurations that will be fully elaborated on elsewhere [63]. The comparison of these results with the experimental binding energy of -127.6 MeV [124] proves that the V_{UCOM} two-body interaction provides an excellent description of ground-state energies for heavier nuclei.

The results of the IT-CI(4p4h) and IT-CI(4p4h)+MRD calculations based on the HF-optimized basis are summarized in Fig. 4(a). With increasing size of the single-particle basis from $e_{\max} = 4$ to 7 the position of the energy minimum shifts systematically toward larger $\hbar\Omega$. The Davidson correction remains on the order of 1 MeV for all model-space sizes and oscillator frequencies, indicating that the effects of beyond-4p4h configurations are small when the HF basis set is employed. A similar picture emerges from the CC calculations, shown in Fig. 4(b), which use the same HF-optimized bases and the same model spaces as the IT-CI(4p4h) and IT-CI(4p4h)+MRD calculations. The inclusion of connected triples through the CR-CC(2,3) scheme leads to a lowering of the ground-state energy by up to 6 MeV, indicating the importance of T_3 cluster contributions in the quantitative calculations of the nuclear binding energies.

A direct comparison of the IT-CI(4p4h)+MRD and CR-CC(2,3) results is presented in Fig. 4(c). The agreement between these two entirely different many-body approaches is extraordinary. Apart from the largest model space employed

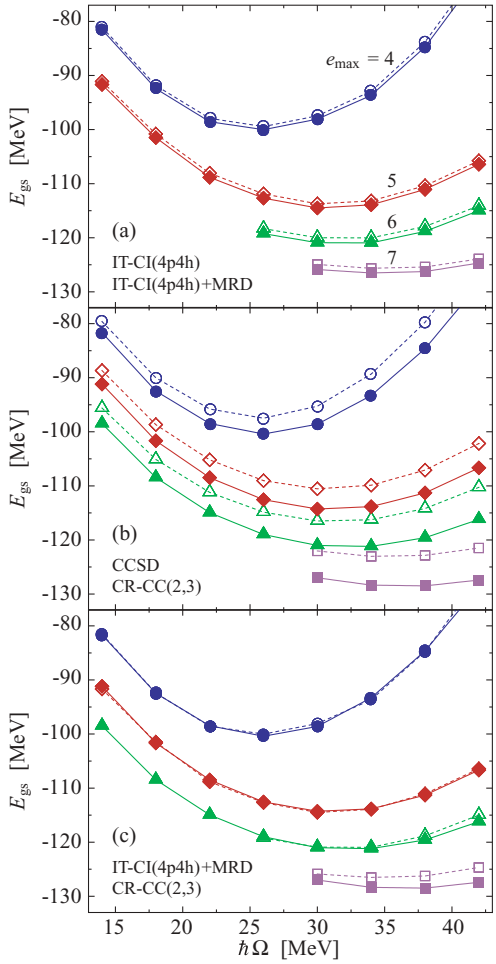

FIG. 4. (Color online) Systematic comparison of IT-CI and CC results for the ground-state energy of ^{16}O using HF-optimized single-particle bases with $e_{max} = 4$, 5, 6, and 7. (a) Comparison of IT-CI(4p4h) (open symbols) with IT-CI(4p4h)+MRD (filled symbols). (b) Comparison of CCSD (open symbols) with CR-CC(2,3) (filled symbols). (c) Comparison of IT-CI(4p4h)+MRD (open symbols) with CR-CC(2,3) (filled symbols).

in this study consisting of eight major oscillator shells, the two data sets are practically on top of each other. For the largest $e_{max} = 7$ space, the discrepancies between the CR-CC(2,3) and IT-CI(4p4h)+MRD results are slightly larger than in the case of smaller basis sets, i.e., the CR-CC(2,3) energies are approximately 1–2 MeV lower than the corresponding IT-CI(4p4h)+MRD energies, but the overall agreement between the IT-CI(4p4h)+MRD and CR-CC(2,3) energies is outstanding. Based on this systematic agreement, we can conclude that neither the lack of strict size extensivity of the truncated IT-CI(4p4h) calculations, which can be taken care of through the use of the Davidson corrections, nor the violation of the variational principle by the CC methods, which is compensated by the high accuracy these methods offer, pose significant practical problems.

The excellent agreement between the CR-CC(2,3) and IT-CI(4p4h)+MRD data can be rationalized by comparing the CC and CI wave function expansions. If we impose the intermediate normalization condition $\langle\Phi_0|\Psi_0\rangle = 1$ exploited in CC theory on the exact CI wave function expansion, we obtain the following relationships between the CI excitation operators C_n and the CC cluster components T_n:

$$C_1 = T_1, \tag{43}$$

$$C_2 = T_2 + \tfrac{1}{2}T_1^2, \tag{44}$$

$$C_3 = T_3 + T_1T_2 + \tfrac{1}{6}T_1^3, \tag{45}$$

$$C_4 = T_4 + T_1T_3 + \tfrac{1}{2}T_2^2 + \tfrac{1}{2}T_1^2T_2 + \tfrac{1}{24}T_1^4, \quad \text{etc.} \tag{46}$$

By design, the CR-CC(2,3) approach provides a highly accurate description of the connected T_1, T_2, and T_3 clusters, but not of T_4 or T_n with $n > 4$, and of all of the disconnected product terms that enter the C_n excitation operators with $n = 1$–4, except for T_1T_3. The T_1T_3 term is much smaller than the leading 4p4h component represented by $(1/2)T_2^2$, particularly when the HF basis is employed. When the HF basis is employed, $(1/2)T_2^2$ contributes to the second-order many-body perturbation theory correction to the wave function and the fourth-order correction to the energy, whereas the lowest-order corrections to the wave function and energy resulting from the T_1T_3 cluster are fourth and sixth, respectively. The connected T_4 cluster contributions, which contribute to the fifth and higher orders in the many-body perturbation theory expansion for the energy, are much smaller than the disconnected $(1/2)T_2^2$ contributions as well. In fact, much of the success of CC theory in areas such as quantum chemistry is related to the fact that one can safely neglect T_4 in calculations for the nondegenerate closed-shell systems. The negligible role of T_4 clusters has also been observed in the study of the semi-closed-shell ^{56}Ni nucleus, as described by the effective Hamiltonian in the pf-shell basis [53]. The ^{16}O nucleus is a closed-shell system, so one does not need T_4 to accurately describe its ground state. This is why the CR-CC(2,3) approach provides a virtually exact description of the CI excitation contributions C_n up to and including the 4p4h (i.e., $n = 4$) terms. Because the CR-CC(2,3) method is based on the idea of correcting the CCSD energy for the leading T_3 contributions and because the CCSD approach describes all higher-than-4p4h excitations that can be represented as products of the T_1 and T_2 clusters, one has to correct the IT-CI(4p4h) energies for the selected higher-than-4p4h correlations via the Davidson corrections to improve the agreement between the IT-CI(4p4h) and CR-CC(2,3) data. This explains why the IT-CI(4p4h)+MRD and CR-CC(2,3) results obtained in this work agree so well.

In order to compare the IT-CI(4p4h)+MRD and CR-CC(2,3) results with the aforementioned converged IT-NCSM calculations, an extrapolation $e_{max} \to \infty$ is necessary. In view of the convergence pattern of the CI and CC results and the fact that our IT-CI(4p4h)+MRD and CR-CC(2,3) data are limited to $e_{max} \leqslant 7$, this extrapolation can only provide a rough estimate. The crude exponential extrapolations based on the total energies obtained with the four different model space sizes with $e_{max} = 4$–7 at fixed $\hbar\Omega = 30$, 34, 38, and 42 MeV, for which the full set of the IT-CI(4p4h)+MRD and CR-CC(2,3) data for $e_{max} = 4$–7 is available, lead to an estimate of the $e_{max} \to \infty$ CR-CC(2,3) energy in the range of -131 to -133 MeV in the entire $\hbar\Omega = 30$–42 MeV region. The IT-CI(4p4h)+MRD result is similar. It looks

as though the $e_{\max} \to \infty$ CR-CC(2,3) energies of -131 to -133 MeV and their IT-CI(4p4h)+MRD analogs, obtained via the above exponential extrapolations based on the total energies, are in excellent agreement with the extrapolated IT-NCSM(4p4h)+MRD result of (-130 ± 1) MeV, but we should be very careful in interpreting this agreement, which might be fortuitous, because crude extrapolations based on the limited set of CC and CI data that we have access to may carry sizable error bars. For example, if we use the more careful approach where instead of extrapolating total energies we extrapolate only the correlation energies obtained with $e_{\max} = 3$, 5, and 7, and add the results to the highly accurate estimate of the converged (to within 0.1 MeV) HF energy resulting from the $e_{\max} = 20$ HF calculations, we obtain the extrapolated total CR-CC(2,3) energy in the range of -135 to -141 MeV in the entire $\hbar\Omega = 30$–42 MeV region. The analogous IT-CI(4p4h)+MRD energies are in the range of -132 to -135 MeV. The use of only odd values of $e_{\max}$ in the correlation energy extrapolations can be justified by the fact that the HF and, in consequence, correlation energies do not change uniformly when increasing the basis set; changes in the HF energies are much stronger when another radial excitation is added to the p states, as observed when going from $e_{\max} = 4$ to 5 and from $e_{\max} = 6$ to 7. Thus, based on the limited set of the CC and CI data we have at our disposal, we can only state that the extrapolated $e_{\max} \to \infty$ CR-CC(2,3) and IT-CI(4p4h)+MRD energies fall within the broader range of -131 to -141 MeV, which implies that our extrapolated results carry an uncertainty which could be as big as about 10 MeV. Clearly, the few MeV differences between the extrapolated CR-CC(2,3)/IT-CI(4p4h)+MRD and IT-NCSM(4p4h)+MRD results for the binding energy of ^{16}O prompt further study, so that we can understand the nature of these differences in more precise terms, but it is already worth pointing out that these few MeV differences between the extrapolated CR-CC(2,3) and IT-CI(4p4h)+MRD binding energies on the one hand and their $N_{\max} \to \infty$ IT-NCSM(4p4h)+MRD counterpart on the other hand are consistent with our estimate of the effect of center-of-mass contaminations on the calculated CR-CC(2,3) and IT-CI(4p4h) energies discussed in Sec. IV A. Because the CR-CC(2,3), IT-CI(4p4h)+MRD, and IT-NCSM(4p4h)+MRD methods contain similar many-body correlation effects as $e_{\max}(N_{\max}) \to \infty$ and because the IT-NCSM(4p4h)+MRD results are virtually free of the center-of-mass contaminations (cf. Sec. IV A), it is quite possible that the center-of-mass contaminations in the CR-CC(2,3) and IT-CI(4p4h)+MRD results are largely responsible for the observed few MeV differences between the extrapolated CR-CC(2,3) or IT-CI(4p4h)+MRD and IT-NCSM(4p4h)+MRD energies. The fact that the relatively inexpensive CR-CC(2,3) approach can produce the binding energy of ^{16}O that differs from the best IT-NCSM(4p4h)+MRD estimate and experiment by only a few MeV (less than 10%), when the V_{UCOM} interaction is employed, is an indication that the CR-CC(2,3) method captures practically all correlations relevant for the description of the ground state of ^{16}O and that V_{UCOM} provides the accurate representation of the relevant nucleon-nucleon interactions.

V. CONCLUSIONS

Through the direct comparison of results for the ^{16}O ground-state energy obtained using the V_{UCOM} interaction within the IT-NCSM, IT-CI, and CC approaches, we have established a comprehensive picture of the quality of the different many-body approaches and the practical relevance of formal limitations associated with each one of them. Among the points that we have discussed in detail are the possible role of center-of-mass contaminations, the choice of the single-particle basis, and the impact of size-extensivity.

The analysis of the coupling of intrinsic and center-of-mass motions using the Lawson prescription shows that the IT-CI and CC methods, which are based on a single-particle truncation when constructing the relevant model spaces, exhibit a coupling between intrinsic and center-of-mass motions that in the case of ^{16}O affects the intrinsic energies at the level of about 2–6 MeV or so when the HO reference determinant is employed. The same analysis also indicates that a small value of the expectation value of the center-of-mass Hamiltonian $\langle H_{\mathrm{c.m.}} \rangle$ alone does not automatically warrant a decoupling and a spuriousness-free intrinsic state. Only the IT-NCSM approach, which is based on approximating the complete $N_{\max}\hbar\Omega$ model space of the NCSM theory, shows a virtually perfect decoupling, leading to effectively contamination-free intrinsic eigenstates. However, the relatively small center-of-mass contaminations observed in the IT-CI and CC calculations for ^{16}O do not seem to be detrimental for the quality of the resulting energies, which almost perfectly agree with one another when the appropriate levels of both theories are employed, namely IT-CI(4p4h)+MRD in the case of IT-CI and CR-CC(2,3) in the case of CC, and which are in reasonable agreement with the results of the converged IT-NCSM(4p4h)+MRD calculations when we attempt to extrapolate the IT-CI(4p4h)+MRD and CR-CC(2,3) results to the complete basis set limit. The remaining few (up to about 10) MeV differences between the crudely extrapolated CR-CC(2,3) and IT-CI(4p4h)+MRD energies and the converged IT-NCSM(4p4h)+MRD calculations are consistent with the magnitude of the center-of-mass contaminations present in the CR-CC(2,3) and IT-CI(4p4h)+MRD calculations.

The comparison of the calculations employing the HO single-particle bases with the calculations using HF-optimized bases demonstrates that the CC method is largely insensitive to the basis set choice, whereas the IT-CI calculations show a strong basis set dependence, significantly benefiting from the use of an optimized basis. This fundamentally different behavior of the CC and IT-CI approaches with regard to the choice of the single-particle basis is related to the presence of the $\exp(T_1)$ component in the exponential wave operator of CC theory, as in the Thouless theorem, which makes the CC results almost insensitive to the basis set choice, and the incomplete treatment of this component by the linear wave operator of IT-CI. As shown in this work, an effective measure of the suitability of the single-particle basis for the truncated CI (e.g., IT-CI) calculations can be provided by the T_1 or C_1 excitation amplitudes and the corresponding T_1 Diagnostic as well as the magnitude of the Davidson extensivity corrections.

The T_1 or C_1 values, the values of the T_1 Diagnostic, and the Davidson extensivity corrections all become large if the basis is ill adapted to the truncated CI calculations of interest. We can, therefore, check the suitability of a given basis set for the IT-CI and IT-NCSM calculations by monitoring these quantities.

When using the HF-optimized basis in large scale CR-CC(2,3) and IT-CI(4p4h)+MRD calculations, we observe an excellent agreement of the ground-state energies of ^{16}O for all values of $\hbar\Omega$ and $e_{\max}$. Only for the largest $e_{\max} = 7$ space and large $\hbar\Omega$ values do we observe the slightly larger differences between the CR-CC(2,3) and IT-CI(4p4h)+MRD results, on the order of 1 to 2 MeV. This excellent agreement between the results of the CR-CC(2,3) and IT-CI(4p4h)+MRD calculations demonstrates that neither the violation of strict size extensivity by the IT-CI schemes nor the violation of the variational principle by the truncated CC schemes are of major practical concern in nuclear structure calculations, because both the IT-CI and CC methodologies are systematically improvable through the inclusion of higher-order many-body components in the corresponding excitation operators (C_m components in the case of IT-CI and cluster components T_m in the case of CC) and the use of suitable energy corrections (the Davidson corrections in the case of IT-CI and the corrections due to the effects of higher-order clusters in CC). The IT-CI(4p4h)+MRD and the CR-CC(2,3) results converge toward somewhat lower binding energies than the IT-NCSM(4p4h)+MRD calculations, but, as already pointed out, the observed few MeV or a few-percentage differences between the extrapolated $e_{\max} \to \infty$ IT-CI(4p4h)+MRD and CR-CC(2,3) energies on the one hand and the $N_{\max} \to \infty$ IT-NCSM(4p4h)+MRD energies on the other hand are consistent with the effects expected from the presence of center-of-mass contaminations in the CI and CC calculations. Based on all of these observations, we conclude that all *ab initio* schemes used in the present work—IT-NCSM, IT-CI, and CC—provide powerful, affordable, and potentially accurate computational tools to tackle the nuclear many-body problem. Due to the complementarity of the IT-NCSM, IT-CI, and CC methods, comparative computational studies using all of these approaches, following the analysis presented in this work, may provide a comprehensive and precise picture of nuclear structure of p-shell nuclei and beyond.

Finally, it is interesting to compare the results for the ground-state energy of ^{16}O obtained in the present study with the V_{UCOM} two-body interaction with the earlier recent CC calculations using other two-body interactions. The extrapolated ground-state energy obtained in the IT-NCSM(4p4h)+MRD calculations with V_{UCOM} is (-130 ± 1) MeV, i.e., within about 2 MeV from the experimental value of -127.6 MeV. Although the CR-CC(2,3) results reported in this work and obtained with the same potential are not as well converged with the single-particle basis set, the attempt to extrapolate the CR-CC(2,3) energies to the $e_{\max} \to \infty$ limit produced the result that implies overbinding, compared to experiment, on the order of 3–13 MeV. We believe that most of this overbinding and the analogous overbinding observed in IT-CI(4p4h)+MRD calculations is due to center-of-mass contaminations that affect the CCSD and the subsequent CR-CC(2,3) calculations as well as the IT-CI(4p4h)+MRD calculations, although future, more detailed, studies will be required to verify this statement. The CR-CCSD(T) study reported in Ref. [48] using the Idaho-A two-body potential [5] produced, after correcting the result for the effect of the Coulomb interaction, an extrapolated ground-state energy of about -109.3 MeV. A similar result (approximately, -112 MeV) was obtained with the two-body component of the chiral N^{3}LO potential [6], which includes the Coulomb interaction directly [48]. Thus, with these chiral two-body interactions, the CR-CCSD(T) approach underbinds ^{16}O by approximately 17 MeV, which was concluded to be due to the effect of missing three-body forces [48]. Similar underbinding has also been observed in the CC calculations for ^{16}O employing the Argonne V18 potential reported in Refs. [44–46], where the explicit inclusion of three-nucleon interactions was used to improve the agreement with experiment [44,45]. A recent CCSD(T) study based on the two-body $V_{\mathrm{low}k}$ interaction presented in Ref. [52] (CCSD(T) is another noniterative treatment of T_3 clusters in CC theory [125], which is less robust and generally less accurate than the CR-CC(2,3) approach used in the present study [87–89,91,94–96,98]), has led to an extrapolated ground-state energy of -148.2 MeV, i.e., the binding energy overestimated by more than 20 MeV. These comparisons demonstrate that the V_{UCOM} interaction, in contrast to many other two-nucleon interactions, requires no or minimal contributions from a three-body force to provide a reasonably accurate description of the ground-state energy of ^{16}O. An extension of these investigations to open-shell systems and excited states, including other p-shell nuclei, will be presented elsewhere.

ACKNOWLEDGMENTS

This work was supported by the Deutsche Forschungsgemeinschaft through contract SFB 634, the Helmholtz International Center for FAIR within the framework of the LOEWE program launched by the State of Hesse (R.R.), the Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, Office of Science, US Department of Energy (Grant No. DE-FG02-01ER15228; P.P) and the National Science Foundation's Graduate Research Fellowship (J.R.G). The coupled-cluster calculations were performed on the computer systems provided by the High Performance Computing Center and Department of Chemistry at Michigan State University.

[1] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).
[2] R. Machleidt, Phys. Rev. C **63**, 024001 (2001).
[3] S. Weinberg, Phys. Lett. **B251**, 288 (1990).
[4] U. van Kolck, Prog. Part. Nucl. Phys. **43**, 337 (1999).
[5] D. R. Entem and R. Machleidt, Phys. Lett. **B524**, 93 (2002).

[6] D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001R (2003).
[7] E. Epelbaum, A. Nogga, W. Glöckle, H. Kamada, Ulf-G. Meißner, and H. Witala, Phys. Rev. C **66**, 064001 (2002).
[8] S. K. Bogner, T. T. S. Kuo, and A. Schwenk, Phys. Rep. **386**, 1 (2003).
[9] S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. C **75**, 061001R (2007).
[10] H. Hergert and R. Roth, Phys. Rev. C **75**, 051001R (2007).
[11] R. Roth, S. Reinhardt, and H. Hergert, Phys. Rev. C **77**, 064003 (2008).
[12] R. Roth, H. Hergert, P. Papakonstantinou, T. Neff, and H. Feldmeier, Phys. Rev. C **72**, 034002 (2005).
[13] R. Roth, T. Neff, H. Hergert, and H. Feldmeier, Nucl. Phys. **A745**, 3 (2004).
[14] H. Feldmeier, T. Neff, R. Roth, and J. Schnack, Nucl. Phys. **A632**, 61 (1998).
[15] T. Neff and H. Feldmeier, Nucl. Phys. **A713**, 311 (2003).
[16] S. C. Pieper and R. B. Wiringa, Annu. Rev. Nucl. Part. Sci. **51**, 53 (2001).
[17] R. B. Wiringa and S. C. Pieper, Phys. Rev. Lett. **89**, 182501 (2002).
[18] S. C. Pieper, K. Varga, and R. B. Wiringa, Phys. Rev. C **66**, 044310 (2002).
[19] S. C. Pieper, R. B. Wiringa, and J. Carlson, Phys. Rev. C **70**, 054325 (2004).
[20] S. C. Pieper, Nucl. Phys. **A751**, 516 (2005).
[21] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000).
[22] P. Navrátil, G. P. Kamuntavicius, and B. R. Barrett, Phys. Rev. C **61**, 044001 (2000).
[23] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. C **62**, 054311 (2000).
[24] E. Caurier, P. Navrátil, W. E. Ormand, and J. P. Vary, Phys. Rev. C **64**, 051301(R) (2001).
[25] P. Navrátil and W. E. Ormand, Phys. Rev. Lett. **88**, 152502 (2002).
[26] B. R. Barrett, P. Navrátil, and J. P. Vary, Nucl. Phys. **A704**, 254C (2002).
[27] E. Caurier, P. Navrátil, W. E. Ormand, and J. P. Vary, Phys. Rev. C **66**, 024314 (2002).
[28] P. Navrátil and W. E. Ormand, Phys. Rev. C **68**, 034305 (2003).
[29] H. Zhan, A. Nogga, B. R. Barrett, J. P. Vary, and P. Navrátil, Phys. Rev. C **69**, 034302 (2004).
[30] M. A. Hasan, J. P. Vary, and P. Navrátil, Phys. Rev. C **69**, 034332 (2004).
[31] J. P. Vary, B. R. Barrett, R. Lloyd, P. Navrátil, A. Nogga, and W. E. Ormand, Nucl. Phys. **A746**, 123C (2004).
[32] B. R. Barrett, P. Navrátil, A. Nogga, W. E. Ormand, and J. P. Vary, Nucl. Phys. **A746**, 579C (2004).
[33] I. Stetcu, B. R. Barrett, P. Navrátil, and J. P. Vary, Phys. Rev. C **71**, 044325 (2005).
[34] J. P. Vary, O. V. Atramentov, B. R. Barrett, M. Hasan, A. C. Hayes, R. Lloyd, A. I. Mazur, P. Navrátil, A. G. Negoita, A. Nogga, W. E. Ormand, S. Popescu, B. Shehadeh, A. M. Shirokov, J. R. Spence, I. Stetcu, S. Stoica, T. A. Weber, and S. A. Zaytsev, Eur. Phys. J. A **25** (Suppl. 1), 475 (2005).
[35] I. Stetcu, B. R. Barrett, P. Navrátil, and J. P. Vary, Phys. Rev. C **73**, 037307 (2006).
[36] A. Nogga, P. Navrátil, B. R. Barrett, and J. P. Vary, Phys. Rev. C **73**, 064002 (2006).
[37] B. R. Barrett, I. Stetcu, P. Navrátil, and J. P. Vary, J. Phys. A: Math. Gen. **39**, 9983 (2006).
[38] P. Navrátil, V. G. Gueorguiev, J. P. Vary, W. E. Ormand, and A. Nogga, Phys. Rev. Lett. **99**, 042501 (2007).
[39] R. Roth and P. Navrátil, Phys. Rev. Lett. **99**, 092501 (2007).
[40] C. Forssen, J. P. Vary, E. Caurier, and P. Navrátil, Phys. Rev. C **77**, 024301 (2008).
[41] E. Caurier, G. Martínez-Pinedo, F. Nowacki, A. Poves, and A. Zuker, Rev. Mod. Phys. **77**, 427 (2005).
[42] D. J. Dean and M. Hjorth-Jensen, Phys. Rev. C **69**, 054320 (2004).
[43] D. J. Dean, J. R. Gour, G. Hagen, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, P. Piecuch, and M. Włoch, Nucl. Phys. **A752**, 299 (2005).
[44] B. Mihaila and J. H. Heisenberg, Phys. Rev. Lett. **84**, 1403 (2000).
[45] B. Mihaila and J. H. Heisenberg, Phys. Rev. C **61**, 054309 (2000).
[46] J. H. Heisenberg and B. Mihaila, Phys. Rev. C **59**, 1440 (1999).
[47] K. Kowalski, D. J. Dean, M. Hjorth-Jensen, T. Papenbrock, and P. Piecuch, Phys. Rev. Lett. **92**, 132501 (2004).
[48] M. Włoch, D. J. Dean, J. R. Gour, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, and P. Piecuch, Phys. Rev. Lett. **94**, 212501 (2005).
[49] M. Włoch, D. J. Dean, J. R. Gour, P. Piecuch, M. Hjorth-Jensen, T. Papenbrock, and K. Kowalski, Eur. Phys. J. A **25** (Suppl. 1), 485 (2005).
[50] M. Włoch, J. R. Gour, P. Piecuch, D. J. Dean, M. Hjorth-Jensen, and T. Papenbrock, J. Phys. G: Nucl. Part. Phys. **31**, S1291 (2005).
[51] J. R. Gour, P. Piecuch, M. Hjorth-Jensen, M. Włoch, and D. J. Dean, Phys. Rev. C **74**, 024310 (2006).
[52] G. Hagen, D. J. Dean, M. Hjorth-Jensen, T. Papenbrock, and A. Schwenk, Phys. Rev. C **76**, 044305 (2007).
[53] M. Horoi, J. R. Gour, M. Włoch, M. D. Lodriguito, B. A. Brown, and P. Piecuch, Phys. Rev. Lett. **98**, 112501 (2007).
[54] J. R. Gour, M. Horoi, P. Piecuch, and B. A. Brown, Phys. Rev. Lett. **101**, 052501 (2008).
[55] R. Langhoff and E. R. Davidson, Int. J. Quantum Chem. **8**, 61 (1974).
[56] H.-J. Werner, Adv. Chem. Phys. **69**, 1 (1987).
[57] P. J. Bruna and S. D. Peyerimhoff, Adv. Chem. Phys. **67**, 1 (1987).
[58] J. Paldus, in *New Horizons of Quantum Chemistry*, edited by P.-O. Löwdin and B. Pullman (Reidel, Dordrecht, 1983), p. 31.
[59] R. Buenker and S. Peyerimhoff, in *New Horizons of Quantum Chemistry*, edited by P.-O. Löwdin and B. Pullman (Reidel, Dordrecht, 1983), p. 183.
[60] P. J. Bruna, S. D. Peyerimhoff, and R. J. Buenker, Chem. Phys. Lett. **72**, 278 (1980).
[61] K. Jankowski, L. Meissner, and J. Wasilewski, Int. J. Quantum Chem. **28**, 931 (1985).
[62] P. G. Szalay and R. J. Bartlett, J. Chem. Phys. **103**, 3600 (1995).
[63] R. Roth, arXiv:0903.4605 [nucl-th] (2009).
[64] R. J. Buenker and S. D. Peyerimhoff, Theor. Chim. Acta **35**, 33 (1974).
[65] R. J. Buenker and S. D. Peyerimhoff, Theor. Chim. Acta **39**, 217 (1975).
[66] P. R. Surján, Z. Rolik, Á. Szabados, and D. Köhalmi, Ann. Phys. (Leipzig) **13**, 223 (2004).
[67] E. A. Hylleraas and B. Undheim, Z. Phys. A **65**, 759 (1930).

[68] W. Duch and G. Diercksen, J. Chem. Phys. **101**, 3018 (1994).
[69] F. Coester, Nucl. Phys. **7**, 421 (1958).
[70] F. Coester and H. Kümmel, Nucl. Phys. **17**, 477 (1960).
[71] J. Čížek, J. Chem. Phys. **45**, 4256 (1966).
[72] J. Čížek, Adv. Chem. Phys. **14**, 35 (1969).
[73] J. Čížek and J. Paldus, Int. J. Quantum Chem. **5**, 359 (1971).
[74] H. Kümmel, J. H. Lührmann, and J. G. Zabolitzky, Phys. Rep. **36**, 1 (1978).
[75] J. Paldus and X. Li, Adv. Chem. Phys. **110**, 1 (1999).
[76] T. D. Crawford and H. F. Schaefer III, Rev. Comput. Chem. **14**, 33 (2000).
[77] P. Piecuch, K. Kowalski, I. S. O. Pimienta, and M. J. McGuire, Int. Rev. Phys. Chem. **21**, 527 (2002).
[78] P. Piecuch, K. Kowalski, I. S. O. Pimienta, P. D. Fan, M. Lodriguito, M. J. McGuire, T. Kucharski, S. A. Kuś, and M. Musiał, Theor. Chem. Acc. **112**, 349 (2004).
[79] R. F. Bishop, in *Microscopic Quantum Many-Body Theories and Their Applications*, Lecture Notes in Physics, Vol. 510, edited by J. Navarro and A. Polls (Springer-Verlag, Berlin, 1998), p. 1.
[80] R. J. Bartlett, in *Modern Electronic Structure Theory*, Part I, edited by D. R. Yarkony (World Scientific, Singapore, 1995), p. 1047.
[81] P. Piecuch and K. Kowalski, in *Computational Chemistry: Reviews of Current Trends*, edited by J. Leszczyński (World Scientific, Singapore, 2000), Vol. 5, p. 1.
[82] H. J. Monkhorst, Int. J. Quantum Chem. Symp. **11**, 421 (1977).
[83] G. D. Purvis and R. J. Bartlett, J. Chem. Phys. **76**, 1910 (1982).
[84] J. M. Cullen and M. C. Zerner, J. Chem. Phys. **77**, 4088 (1982).
[85] G. E. Scuseria, A. C. Scheiner, T. J. Lee, J. E. Rice, and H. F. Schaefer III, J. Chem. Phys. **86**, 2881 (1987).
[86] P. Piecuch and J. Paldus, Int. J. Quantum Chem. **36**, 429 (1989).
[87] P. Piecuch and M. Włoch, J. Chem. Phys. **123**, 224105 (2005).
[88] P. Piecuch, M. Włoch, J. R. Gour, and A. Kinal, Chem. Phys. Lett. **418**, 467 (2006).
[89] M. Włoch, J. R. Gour, and P. Piecuch, J. Phys. Chem. A **111**, 11359 (2007).
[90] K. Kowalski and P. Piecuch, J. Chem. Phys. **113**, 18 (2000).
[91] M. Włoch, M. D. Lodriguito, P. Piecuch, and J. R. Gour, Mol. Phys. **104**, 2149 (2006).
[92] C. J. Cramer, M. Włoch, P. Piecuch, C. Puzzarini, and L. Gagliardi, J. Phys. Chem. A **110**, 1991 (2006); [Erratum-*ibid.* **111**, 4871 (2007)].
[93] C. J. Cramer, A. Kinal, M. Włoch, P. Piecuch, and L. Gagliardi, J. Phys. Chem. A **110**, 11557 (2006); [Erratum-*ibid.* **111**, 4871 (2007)].
[94] A. Kinal and P. Piecuch, J. Phys. Chem. A **111**, 734 (2007).
[95] Y. Ge, M. S. Gordon, and P. Piecuch, J. Chem. Phys. **127**, 174106 (2007).
[96] P. Piecuch, M. Włoch, and A. J. C. Varandas, Theor. Chem. Acc. **120**, 59 (2008).
[97] J. Zheng, J. R. Gour, J. J. Lutz, M. Włoch, P. Piecuch, and D. G. Truhlar, J. Chem. Phys. **128**, 044108 (2008).
[98] Y. Z. Song, A. Kinal, P. J. S. B. Caridade, A. J. C. Varandas, and P. Piecuch, J. Mol. Struct.: THEOCHEM **859**, 22 (2008).
[99] C. J. Cramer, J. R. Gour, A. Kinal, M. Włoch, P. Piecuch, A. R. M. Shahi, and L. Gagliardi, J. Phys. Chem. A **1112**, 3754 (2008).
[100] J. J. Lutz and P. Piecuch, J. Chem. Phys. **128**, 154116 (2008).
[101] T. Van Voorhis and M. Head-Gordon, J. Chem. Phys. **113**, 8873 (2000).
[102] M. Head-Gordon, T. Van Voorhis, S. R. Gwaltney, and E. F. C. Byrd, in *Low-Lying Potential Energy Surfaces*, ACS Symposium Series, Vol. 828, edited by M. R. Hoffmann and K. G. Dyall (American Chemical Society, Washington, D.C., 2002), p. 93.
[103] J. Noga and R. J. Bartlett, J. Chem. Phys. **86**, 7041 (1987); [Erratum-*ibid.* **89**, 3401 (1988)].
[104] G. E. Scuseria and H. F. Schaefer, Chem. Phys. Lett. **152**, 382 (1988).
[105] J. F. Stanton and R. J. Bartlett, J. Chem. Phys. **98**, 7029 (1993).
[106] P. Piecuch and R. Bartlett, Adv. Quantum Chem. **34**, 295 (1999).
[107] P. Piecuch, M. Włoch, J. R. Gour, D. J. Dean, M. Hjorth-Jensen, and T. Papenbrock, in *Nuclei and Mesoscopic Physics: Workshop on Nuclei and Mesoscopic Physics WNMP 2004*, AIP Conference Proceedings, Vol. 777, edited by V. Zelevinsky (AIP, Melville, NY, 2005), p. 28.
[108] A. E. Kondo, P. Piecuch, and J. Paldus, J. Chem. Phys. **102**, 6511 (1995).
[109] M. Włoch, J. R. Gour, K. Kowalski, and P. Piecuch, J. Chem. Phys. **122**, 214107 (2005).
[110] S. A. Kucharski and R. J. Bartlett, Theor. Chim. Acta **80**, 387 (1991).
[111] P. Pulay, Chem. Phys. Lett. **73**, 393 (1980).
[112] G. E. Scuseria, T. J. Lee, and H. F. Schaefer, III, Chem. Phys. Lett. **130**, 236 (1986).
[113] R. Roth, P. Papakonstantinou, N. Paar, H. Hergert, T. Neff, and H. Feldmeier, Phys. Rev. C **73**, 044312 (2006).
[114] P. K. Rath, A. Faessler, H. Müther, and A. Watts, J. Phys. G: Nucl. Part. Phys. **16**, 245 (1990).
[115] I. Moliner, N. R. Walet, and R. F. Bishop, J. Phys. G **28**, 1209 (2002).
[116] R. F. Bishop, M. F. Flynn, M. C. Bosca, E. Buendia, and R. Guardiola, Phys. Rev. C **42**, 1341 (1990).
[117] D. Gloeckner and R. Lawson, Phys. Lett. **B53**, 313 (1974).
[118] F. Palumbo, Nucl. Phys. **A99**, 100 (1967).
[119] D. J. Thouless, Nucl. Phys. **21**, 225 (1960).
[120] E. A. Salter, H. Sekino, and R. J. Bartlett, J. Chem. Phys. **87**, 502 (1987).
[121] T. J. Lee and P. R. Taylor, Int. J. Quantum Chem. **S23**, 199 (1989).
[122] E. Caurier and F. Nowacki, Acta Phys. Pol. B **30**, 705 (1999).
[123] From the set of five results we extract all possible subsets of three data points and perform the extrapolations. The average of the extrapolation results is quoted as energy and the standard deviation as error. Improved IT-NCSM calculations for larger model spaces are reported in Ref. [63] and yield slightly lower extrapolated energies.
[124] G. Audi and A. Wapstra, Nucl. Phys. **A595**, 409 (1995).
[125] K. Raghavachari, G. W. Trucks, J. A. Pople, and M. Head-Gordon, Chem. Phys. Lett. **157**, 479 (1989).