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Computing the dipole polarizability of $^{48}\text{Ca}$ with increased precision

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We compute the electric dipole polarizability of $^{48}\text{Ca}$ with an increased precision by including more correlations than in previous studies. Employing the coupled-cluster method we go beyond singles and doubles excitations and include leading-order three-particle-three-hole (3p-3h) excitations for the ground state, excited states, and the similarity transformed operator. We study electromagnetic sum rules, such as the bremsstrahlung sum rule $\alpha_0$ and the polarizability sum rule $\alpha_D$ using interactions from chiral effective field theory. To gauge the quality of our coupled-cluster approximations we perform several benchmarks with the effective interaction hyperspherical harmonics approach in $^4\text{He}$ and with self consistent Green’s function in $^{40}\text{O}$. We compute the dipole polarizability of $^{48}\text{Ca}$ employing the chiral interaction $N^\text{3LO}_{\text{sat}}$ [Ekström et al., Phys. Rev. C 91, 051301 (2015)] and the 1.8/2.0 (EM) [Hebeler et al., Phys. Rev. C 83, 031301 (2011)]. We find that the effect of 3p-3h excitations in the ground state is small for 1.8/2.0 (EM) but non-negligible for $N^\text{3LO}_{\text{sat}}$. The addition of these new correlations allows us to improve the precision of our $^{48}\text{Ca}$ calculations and reconcile the recently reported discrepancy between coupled-cluster results based on these interactions and the experimentally determined $\alpha_D$ from proton inelastic scattering in $^{48}\text{Ca}$ [Birkhan et al., Phys. Rev. Lett. 118, 252501 (2017)]. For the computation of electromagnetic and polarizability sum rules, the inclusion of leading-order 3p-3h excitations in the ground state is important, while less so for the excited states and the similarity-transformed dipole operator.

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I. INTRODUCTION

The electric dipole polarizability $\alpha_D$ has been measured in several nuclei [1–4], and is of key interest to theorists. On the one hand, mean-field calculations suggest that $\alpha_D$ is strongly correlated to the neutron skin, i.e. the difference between the root-mean-square (RMS) radii of the neutron and proton distributions [5–10], and thereby connects nuclei and neutron stars [11]. On the other hand, computations of $^{48}\text{Ca}$ by Hagen et al. [12] based on Hamiltonians from chiral effective field theory [13–14] exhibit no correlations between the neutron skin and $\alpha_D$, but do correlate the latter with both the RMS radius of the neutron distribution and the symmetry energy (and its slope) in nuclear matter, again providing a connection between neutron-star physics and finite nuclei [15–16].

The prediction [12] and measurement [4] of the dipole polarizability in $^{48}\text{Ca}$ agree within uncertainties, but theory somewhat overestimates the experimental data for some interactions. This motivates us to revisit this nucleus in this work, with an emphasis on computing $\alpha_D$ more precisely by going to the next level of approximation and include more many-body correlations.

We note that the study of the role of many-body correlations, while performed here with the coupled-cluster method [17–23], is relevant also for other methods such as self consistent Green’s functions [24], in-medium similarity renormalization group [25–26], and Gorkov-Green’s function approaches [27]. All these methods seek economical ways to include the necessary particle-hole correlations required to achieve a precise calculation of energies and observables of ground- and excited states [28–30]. Thus, we expect that our results will also be useful for those applications.

In the last decade, major advancements have been made in first principles approaches to nuclear structure [23–26, 31–35]. Realistic descriptions of nuclei as heavy as $^{78}\text{Ni}$ and $^{100}\text{Sn}$ have recently been achieved based on state-of-the-art nucleon-nucleon ($NN$) and three-nucleon forces (3NFs) from chiral effective field theory [36–38]. This advancement is based on the combination of first principles methods that scale poly-
In practice, one often inserts completeness relations on bremsstrahlung sum rule and focuses on a few well-known sum rules, namely the of the nucleus. In this paper, we will take this approach moments one can gain useful insights into the dynamics knowing all of its (existing) moments, already from a few observables within coupled-cluster theory using various approximation levels, and infer information on the nuclear dynamics from a comparison to other available theoretical computations and/or experimental data.

In the long wave-length approximation, i.e., in the limit of \( q \to 0 \), the electric dipole operator reads

\[
\hat{\Theta} = \sum_k^A (r_k - R_{cm}) \left( \frac{1 + r_k^3}{2} \right).
\]

Here \( r_k \) and \( R_{cm} \) are the coordinates of the \( k \)-th nucleon and the center of mass of the nucleus, respectively, and \( r_k^3 \) is the third component of the isospin operator. As an example, the photo-disintegration cross section of a nucleus below the pion production threshold becomes

\[
\sigma_\gamma(\omega) = 4\pi^2 a_\omega R(\omega).
\]

Here \( R(\omega) \) is the response function \([1]\) of the translationally invariant dipole operator \([4]\) for \( \omega = |q| \). Employing an \( NN \) interaction from chiral effective field theory \([65]\), this reaction cross section was calculated in Refs. \([68, 69]\) using coupled-cluster theory with singles and doubles excitations (CCSD). While those calculations agreed with experimental data for \(^{4}\text{He}, \ ^{16,22}\text{O}\) and \(^{40}\text{Ca}\), they lacked a better understanding of uncertainties related to the underlying Hamiltonian and the applied many-body approach.

The computation of a cross section or related sum rule exhibits various theoretical uncertainties. Often, the largest uncertainty results from truncations of the employed chiral effective field theory at some given order in the power counting, whereas statistical uncertainties due to the optimization of the interaction are significantly smaller \([50, 66, 67]\). While a robust quantification of systematic uncertainties related to the employed chiral interactions is still lacking, a rough estimate can be made by employing a large set of different chiral interactions \([38, 48, 60, 68, 69]\). Uncertainties from finite harmonic-oscillator basis can be estimated by varying the number of oscillator shells \( N_{\text{max}} \) and the oscillator frequency \( (h\Omega) \). We found that this uncertainty is of the order of 1\% for calculations in nuclei with mass number up to \( A = 48 \). Another source of uncertainty in the coupled-cluster method comes from truncating the cluster operator at some low-order particle-hole excitation rank. Previous works employed the CCSD approximation, and neglected higher order excitations, such as \( 3p-3h \) excitations. It is the purpose of this paper to investigate the role of leading-order \( 3p-3h \) excitations in the ground state, excited states, and the similarity transformed operator in the calculation of the bremsstrahlung sum rule \( m_0 \) \([70, 73]\) and on the electric dipole polarizability sum rule \( \alpha_D \) \([74]\).

The electric dipole polarizability is related to the inverse energy weighted sum rule \( m_{-1} \) as

\[
\alpha_D = 2\alpha \int_{\omega_{\text{ex}}}^{\infty} d\omega \frac{R(\omega)}{\omega} = 2\alpha \ m_{-1}.
\]
Due to the inverse energy weight, this sum rule is more sensitive to the low-energy part of the excitation spectrum.

This paper is organized as follows. In Section II we introduce the formalism used to calculate the response functions, and the sum rules $m_0$ and $\alpha_D$. We also present the nomenclature used for the various approximation schemes that we implemented in this work. In Section III we present benchmarking results for $m_0$ and $\alpha_D$ in $^3$He and $^{16}$O to validate our approach. In Section IV, we revisit our $^{48}$Ca calculations and compare them with the recent experimental data of Ref. [4]. Finally, we draw our conclusions in Section V.

II. THEORETICAL METHODS

Coupled-cluster theory \[17, 19, 20, 22, 23, 40, 75–77\] is based on the similarity transformed Hamiltonian,
\[
\overline{H}_N = e^{-T} H_N e^{T}, \quad T = T_1 + T_2 + T_3 \ldots
\] (7)

Here $H_N$ is normal-ordered with respect to a single-reference state $|\Phi_0\rangle$ (usually the Hartree-Fock state), and $T$ is an expansion in particle-hole excitations with respect to this reference. The similarity transformation decouples all particle-hole excitations from the ground state, and the reference state $|\Phi_0\rangle$ becomes the exact ground state of $\overline{H}_N$. In practice, the operator $T$ is truncated at some low rank particle-hole excitation level. The similarity transformed Hamiltonian can be evaluated using the Baker-Campbell-Hausdorff expansion, and terminates at doubly nested commutators for a normal-ordered Hamiltonian containing at most up to two-body terms. The drawback from having an exactly terminating commutator expansion, is that the similarity transformed Hamiltonian is non-Hermitian and thus requires the computation of both the left and right eigenstates in order to evaluate expectation values and transitions. The left ground state is parameterized as
\[
\langle \Psi_0 | = \langle \Phi_0 | (1 + \Lambda), \quad \Lambda = \Lambda_1 + \Lambda_2 + \Lambda_3 \ldots,
\] (8)

where $\Lambda$ is a sum of particle-hole de-excitation operators. The ground-state energy $E_0$ is given by the energy-functional
\[
E_0 = E_{HF} + \langle \Phi_0 | (1 + \Lambda) \overline{H}_N | \Phi_0 \rangle.
\] (9)

Here $E_{HF}$ is the Hartree-Fock reference energy. The left and right ground states are normalized according to $\langle \Phi_0 | (1 + \Lambda) | \Phi_0 \rangle = 1$.

For excited states we employ the equation-of-motion (EOM) coupled-cluster method \[78\] and calculate the right and left excited state of $\overline{H}_N$, i.e.,
\[
\langle \Phi_0 | L_\mu, \overline{H}_N = E_\mu \langle \Phi_0 | L_\mu.
\] (10)

Here $R_\mu$ and $L_\mu$ are linear expansions in particle-hole excitations with
\[
R_\mu = r_0 + \sum_{i,a} r_{ia}^a \hat{a}_i^a \hat{a}_i + \frac{1}{(2\pi)^2} \sum_{i,j,a,b} r_{ia}^a \hat{a}_i^a \hat{a}_j^b \hat{a}_j^b
+ \frac{1}{(3!)^2} \sum_{i,j,k,a,b,c} r_{ij,k}^{abc} \hat{a}_i^a \hat{a}_j^b \hat{a}_k^c \hat{a}_k^c
+ \frac{1}{(4!)^2} \sum_{i,j,k,l,a,b,c,d} r_{ijkl}^{abcd} \hat{a}_i^a \hat{a}_j^b \hat{a}_k^c \hat{a}_l^d \hat{a}_k^c \hat{a}_l^d \hat{a}_k^c \hat{a}_l^d
+ \ldots.
\] (11)

The expression for $L_\mu$ is equivalent. Here, $\hat{a}^\dagger$ and $\hat{a}$ are creation and annihilation operators, respectively. Indices $a, b, c, d$ run over unoccupied orbitals, while $i, j, k, l$ run over occupied orbitals. The left and right excited states are normalized according to
\[
\langle \Phi_0 | L_\mu R_\mu | \Phi_0 \rangle = \delta_{\mu,\mu'}.
\] (13)

The electromagnetic transition strength from the ground to an excited state is evaluated in coupled-cluster theory as
\[
|\langle \Psi_\mu | \hat{\Theta} \Psi_0 \rangle |^2 = \langle \Psi_\mu | \hat{\Theta} \Psi_0 \rangle \langle \Psi_\mu | \hat{\Theta} \Psi_0 \rangle = \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N \overline{R}_\mu | \Phi_0 \rangle \langle \Phi_0 | L_\mu \overline{\Theta}_N | \Phi_0 \rangle.
\] (14)

Here $\overline{\Theta}_N = e^{-T} \Theta_N e^{T}$ is the similarity transformed normal-ordered operator, which in this work is taken to be the electric dipole of Eq. (I). Because it is a one-body operator, the Baker-Campbell-Hausdorff expansion $\overline{\Theta}_N$ terminates at doubly nested commutators
\[
\overline{\Theta}_N = \Theta_N + [\Theta_N, T] + \frac{1}{2}[[\Theta_N, T], T].
\] (15)

Having defined the ground and excited states, we can rewrite the response function in the coupled-cluster formalism starting from Eq. (I) as
\[
R(\omega) = \sum_\mu \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N \overline{R}_\mu | \Phi_0 \rangle \langle \Phi_0 | L_\mu \overline{\Theta}_N | \Phi_0 \rangle \times \delta(E_\mu - E_0 - \omega).
\] (16)

By integrating over the energy $\omega$ we obtain the bremsstrahlung sum rule $m_0$
\[
m_0 = \sum_\mu \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N \overline{R}_\mu | \Phi_0 \rangle \langle \Phi_0 | L_\mu \overline{\Theta}_N | \Phi_0 \rangle.
\] (17)

Using the closure relation we obtain the equivalent expression
\[
m_0 = \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N \cdot \overline{\Theta}_N | \Phi_0 \rangle.
\] (18)

In practice one solves for Eq. (18) by inserting a complete set on the Fock space defined by
\[
1 | \Phi_0 \rangle = \sum_S | S \rangle (S) + \sum_D | D \rangle (D) + \sum_T | T \rangle (T) + \sum_Q | Q \rangle (Q) + \ldots
\] (19)
Here $S, D, T, Q$ label single, double, triple, and quadruple (and so on) excited reference states, corresponding to

$$
\sum_S \langle S | S \rangle = \sum_{ia} \langle \Phi_i^a | \Phi_i^a \rangle ,
$$

$$
\sum_D \langle D | D \rangle = \sum_{ijab} \langle \Phi_{ij}^{ab} | \Phi_{ij}^{ab} \rangle ,
$$

$$
\sum_T \langle T | T \rangle = \sum_{ijkabc} \langle \Phi_{ijk}^{abc} | \Phi_{ijk}^{abc} \rangle ,
$$

$$
\sum_Q \langle Q | Q \rangle = \sum_{ijklabcd} \langle \Phi_{ijkl}^{abcd} | \Phi_{ijkl}^{abcd} \rangle ,
$$

... = ....

Here, $| \Phi_{i_1 \ldots i_n}^{a_1 \ldots a_n} \rangle = a_{i_1}^\dagger \ldots a_{i_n}^\dagger \hat{a}_{i_1} \ldots \hat{a}_{i_n} | \Phi_0 \rangle$ is a np-nh state. Inserting the completeness (19) into Eq. (18) one obtains

$$
m_0 = \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N | \Phi_0 \rangle = \sum_S \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N | S \rangle \langle S | \overline{\Theta}_N | \Phi_0 \rangle
$$

$$
+ \sum_D \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N | D \rangle \langle D | \overline{\Theta}_N | \Phi_0 \rangle
$$

$$
+ \sum_T \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N | T \rangle \langle T | \overline{\Theta}_N | \Phi_0 \rangle
$$

$$
+ \sum_Q \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N | Q \rangle \langle Q | \overline{\Theta}_N | \Phi_0 \rangle + ....
$$

Here the first term is identically zero for non-scalar operators $\Theta$, such as the electric dipole operator considered in this work. Calculating $m_0$ from Eq. (21) is significantly simpler than starting from Eq. (17) since no knowledge of the excited states of $\overline{H}_N$ is required. As a proof of principle we verified that solving Eq. (21) is equivalent to calculating the response function and integrating in $\omega$ using Eq. (17).

The inverse-energy-weighted-polarizability sum rule $\alpha_D$ of Eq. (6) can be calculated by utilizing the Lanczos continued fraction method (79) as

$$
\alpha_D = 2\alpha \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N | \Phi_0 \rangle - \frac{1}{\overline{H}_N - E_0} \overline{\Theta}_N | \Phi_0 \rangle
$$

$$
= 2\alpha \mathcal{I}_L(\sigma = 0, \Gamma = 0)
$$

$$
= m_0 x_{00} .
$$

(22)

Here $\mathcal{I}_L(\sigma, \Gamma)$ is the Lorentz integral transform, and $x_{00}$ is a continued fraction of the Lanczos coefficients. To calculate the Lorentz integral transform (57, 58), one needs to solve an EOM with a source term and the non-symmetric Lanczos algorithm is implemented by constructing the right and left normalized pivots as (see Ref. [79] for details)

$$
| P_r | = \overline{\Theta}_N | \Phi_0 \rangle ,
$$

$$
| P_l | = m_0^{-1} \langle \Phi_0 | (1 + \Lambda) \overline{\Theta}_N^\dagger ,
$$

(23)

(24)

respectively.

So far we have not introduced any approximations in the coupled-cluster formulations for ground and excited states. The most commonly used approximation for the ground state is CCSD (i.e., $T = T_1 + T_2$, and $\Lambda = \Lambda_1 + \Lambda_2$), which typically amounts for about 90% of the full correlation energy in systems with well defined single-reference character [21]. In the following we will denote the CCSD approximation in short with $D$. We will also go beyond the CCSD level by including leading-order 3p-3h excitations using the CCSDT-1 approach [80]. CCSDT-1 is a good approximation to the full CCSDT approach and accounts for about 99% of the correlation energy. In brief, CCSDT-1 is an iterative approach that includes the leading-order contribution ($H N T_2 C$ (here the index $C$ denotes that only connected terms contribute [81]) to the $T_3$ amplitudes with an energy denominator given by the Hartree-Fock single-particle energies, while all $T_3$ contributions to the $T_1$ and $T_2$ amplitudes are fully included.

We will also solve for the corresponding left ground state in the CCSDT-1 following Ref. [82]. To simplify the notation, in the following we will label the CCSDT-1 approximation with $T$. The corresponding approximations we will employ for excited states given in Eq. (10) includes up to 2p-2h in the EOM-CCSD approach, and leading-order 3p-3h excitations in the EOM-CCSDT-1 approach [82] [83]. Because the calculation of $m_0$ and $\alpha_D$ requires a particle-hole expansion of the ground state ($T$ and $\Lambda$) and one for excited states [$R_0$ and $L_0$ for $\alpha_D$ or Eq. (21) for $m_0$], we need to label both of them appropriately. In this work we will investigate different approximation levels in both the ground and excited states.

In order to keep the notation concise we therefore denote each scheme with a pair of labels (separated by a ‘/’ symbol), with the largest order of correlation included in the ground state on the left, and the largest order of correlation included in the excited states on the right as shown in Table I. In the previous work on dipole strengths and polarizabilities [41, 58, 79] both ground and excited states were approximated at the CCSD level, an approximation we label by $D/D$ in this work.

<table>
<thead>
<tr>
<th>ground state</th>
<th>EOM</th>
<th>label</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>S</td>
<td>D/S</td>
</tr>
<tr>
<td>D</td>
<td>D</td>
<td>D/D</td>
</tr>
<tr>
<td>T-1</td>
<td>S</td>
<td>T-1/S</td>
</tr>
<tr>
<td>T-1</td>
<td>D</td>
<td>T-1/D</td>
</tr>
<tr>
<td>T-1</td>
<td>T-1</td>
<td>T-1/T-1</td>
</tr>
</tbody>
</table>

Examining the similarity transformed one-body operator $\overline{\Theta}_N$ of Eq. (15) reveals that for $T = T_1 + T_2$, the expansions of Eqs. (21) and (22) terminate at triply excited determinants ($| T \rangle$). If one includes $T = T_1 + T_2 + T_3$.
the expansions terminate at quadruply excited determinants. Thus, the inclusion of 3p-3h excitations in the ground and excited states requires the implementation of a number of new coupled-cluster diagrams. As usual, we checked such diagrams by comparing the $j$-coupling and $m$-coupling schemes (see, e.g., Ref. [81]).

III. VALIDATION AND BENCHMARKING

For a validation of our approach, we benchmark our results on $^4$He and $^{16}$O. In all the results presented in this Section, $^4$He is calculated with the chiral $NN$ interaction at next-to-next-to-next-to-leading order (N$^3$LO) from Ref. [69], and $^{16}$O is calculated using the N$^2$LO$_{sat}$ interaction [48]. The choice of interaction for $^4$He is motivated by the fact that we want to benchmark the various approximation schemes against virtually exact results from the effective hyperspherical harmonics approach [85], which cannot easily employ the N$^2$LO$_{sat}$ due to the non-locality of the 3NF. For $^{16}$O, the inclusion of 3NFs is necessary for a realistic description of the charge radius and observables correlated with it, such as $m_0$ and $\alpha_D$ [4, 60, 79]. This makes the interaction N$^2$LO$_{sat}$ a good choice. Using this interaction also allows us to benchmark with self consistent Green’s function results [30].

We first explore how the similarity-transformed transition operator depends on the truncation level of included triples excitations. Then we compute the $m_0$ sum rule and the dipole polarizability for $^4$He and $^{16}$O. For $^{16}$O we also show a comparison of running sum rules and discretized responses, which allow us to monitor how excited states move as a function of energy for the various approximation schemes.

A. The similarity transformed transition operator

In the T-1/S, T-1/D, and T-1/T-1 approximations, $T_3$ contributions are included in the one- and two-body parts of the similarity transformed Hamiltonian, while three-body parts from $T_3$ are only included via $(F_NT_3)_C$ (here $F_N$ is the normal ordered one-body Fock matrix). By treating the similarity transformation of a normal-ordered one-body operator $\Theta_N$ consistently with the similarity-transformed Hamiltonian, one has

$$\Theta_N = \left[\Theta_N e^{T_1+T_2+T_3}\right]_C = \overline{\Theta}^D_N + \left[\Theta_N \left(\frac{T_2^2}{2} + T_3 + T_1 T_3\right)\right]_C \quad (25)$$

$$\approx \overline{\Theta}^D_N + \left[\Theta_N \left(\frac{T_2^2}{2}\right)\right]_C \quad (26)$$

$$\approx \overline{\Theta}^D_N \quad (27)$$

where the $C$ index again denotes connected diagrams [81] and $\overline{\Theta}^D_N$ is the similarity-transformed operator in the D approximation. Due to the hierarchy among correlations, one can expect that the terms in Eq. (25) that contain $T_3$ are sub-leading with respect to the $T_2$ term. These terms are also computationally much more demanding since they involve calculating and storing $T_3$ configurations (see Ref. [84] for full expressions). Thus, it is convenient to explore their relevance with respect to using Eq. (26), or even just using Eq. (27), where the operator is similarity transformed as in the D approximation.

In this paper we compute observables by including 3p-3h excitations in the ground and excited states as well as in the similarity transformed operator, and benchmark the various approximations for $\overline{\Theta}_N$ in $^4$He and $^{16}$O, as shown in Table II. We see that for both $m_0$ and $\alpha_D$, the additional terms in Eqs. (25) and (26) have a negligible contribution with respect to Eq. (27), amounting to a sub-percent effect of about 0.2 and 0.7%, respectively. This finding is important in the light of performing computations of heavy nuclei, where calculations with Eq. (27) are more tractable, while using Eq. (25) would be substantially more computationally demanding. Consequently, when calculating $^{48}$Ca in Section IV we will use Eq. (27).

<table>
<thead>
<tr>
<th></th>
<th>$^4$He(a)</th>
<th>$^{16}$O(b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_0$ [fm$^2$]</td>
<td>0.951</td>
<td>4.87</td>
</tr>
<tr>
<td>$\alpha_D$ [fm$^3$]</td>
<td>0.950</td>
<td>4.92</td>
</tr>
<tr>
<td>$m_0$ [fm$^2$]</td>
<td>0.949</td>
<td>4.90</td>
</tr>
<tr>
<td>$\alpha_D$ [fm$^3$]</td>
<td>0.808</td>
<td>0.528</td>
</tr>
<tr>
<td>$m_0$ [fm$^2$]</td>
<td>0.811</td>
<td>0.527</td>
</tr>
</tbody>
</table>

Note that when using Eq. (27) in the calculation of $m_0$ in the T-1/T-1 approximation, 3p-3h excitations enter only in the ground state [see Eq. (18)], and therefore this corresponds to the T-1/D approximation. On the contrary, triples would enter both in the ground and excited states in a calculation of $\alpha_D$, for which T-1/T-1 and T-1/D are different.

B. $^4$He

We now focus on $^4$He and explore the convergence in terms of the model space size $N_{\text{max}}$ for two approximation schemes that includes 3p-3h excitations, namely T-1/T-1 and T-1/D, and compare it to the D/D approximation.

Fig. 1 shows the convergence of $m_0$ and $\alpha_D$ in $^4$He with respect to $N_{\text{max}}$ for $\hbar \Omega = 26$ MeV. Calculations in the T-
FIG. 1. (Color online) Convergence of $m_0$ (a) and $\alpha_D$ (b) for $^4\text{He}$ with respect to the model-space size $N_{\text{max}}$ for $\hbar\Omega = 26$ MeV. Two triples approximations schemes T-1/T-1 (green diamonds) and T-1/D (red circles) are compared to the D/D case (blue squares). The similarity transformed operator is implemented with Eq. (26) and (27), in T-1/T-1 and T-1/D, respectively.

We see that for $m_0$, the results obtained within the T-1/D approximation are close to those obtained in T-1/T-1 approximation. The slight difference stems from the fact that the T-1/T-1 calculations are performed with the similarity transformed operator given in Eq. (26), while T-1/D results are obtained with Eq. (27). We implement these two different equations to graphically show that our findings presented in Table II are consistent in various model spaces and approximations. For $\alpha_D$ we observe a slightly larger difference between the T-1/T-1 and T-1/D approximations, due to the fact that 3p-3h excitations enter in the calculations of excited states as well. Overall, the effects of 3p-3h excitations in $^4\text{He}$ are small, amounting to about 1.5%.

It is now interesting to compare the various coupled-cluster results with respect to the hyperspherical harmonics benchmark values [55, 55] for $^4\text{He}$. Figure 2 shows $m_0$ (a) and $\alpha_D$ (b) obtained for various approximations in coupled-cluster theory: D/D (blue/left), the T-1/D (red/central) and the T-1/T-1 (green/right). The widths of the bands reflect the residual $\hbar\Omega$ dependence for the largest model space $N_{\text{max}} = 14$. The black line is the virtually exact calculation from hyperspherical harmonics expansions using the same interaction. The D/D calculations already get close to the hyperspherical harmonics result, and the addition of 3p-3h correlations in both the T-1/D and T-1/T-1 approaches further improves the agreement for $m_0$. For $\alpha_D$ the T-1/D calculation agrees better with the hyperspherical harmonics result than the T-1/T-1 approach. The overall effect of 3p-3h excitations is small. This benchmark with hyperspherical harmonics suggests that the T-1/D scheme is to be preferred for electromagnetic and polarizability sum rules, and that the inclusion of 3p-3h correlations in the ground state plays a more significant role than the corresponding one in the excited states.

C. $^{16}\text{O}$

Let us turn to $^{16}\text{O}$. First, we check the convergence of the $m_0$ sum rule with respect to the number of 3p-3h configurations included in our calculations. Going beyond the D/D approximation and including 3p-3h excitations in the T-1/S, T-1/D, and T-1/T-1 approaches, the computational cost grows significantly both in terms of number of computational cycles and memory associated with storage of the amplitudes. The computational cost associated with the most expensive term in the D/D approximation is given by $n_{\sigma}^2 n_{u}^4$, while in the T-1/S, T-1/D, and T-1/T-1 approaches it is $n_{\sigma}^2 n_{\sigma}^4$. Here $n_{\sigma}$ is the number of occupied orbitals in the reference state $|\Phi_0\rangle$ and $n_{u}$ is the number of unoccupied orbitals. Clearly, the computational load grows rapidly with the mass of the nucleus ($n_{u} = A$) and the model-space size ($n_{\sigma} \propto N_{\text{max}}^3$). In or-
order to overcome this computational hurdle in the T-1/S, T-1/D, and T-1/T-1 approaches, we introduce an energy cut \( E_{3\text{max}} \) on the allowed \( 3p-3h \) excitations. The truncated space that we employ for the \( 3p-3h \) excitations are thus given by \(|N_a - N_F| + |N_b - N_F| + |N_c - N_F| \leq E_{3\text{max}}\) and \(|N_b - N_F| + |N_c - N_F| \leq E_{3\text{max}}\) with \( N_p = 2n_p + l_p \) being the harmonic-oscillator shell and \( N_F \) the harmonic-oscillator shell at the Fermi surface. The top of Fig. 3 shows the convergence with respect to \( E_{3\text{max}} \) for \( m_0 \) in \(^{16}\text{O}\). We observe that truncating \( E_{3\text{max}} \) to 14 yield results for \(^{16}\text{O}\) that are converged at the 1%-level. Unless stated otherwise, in the remainder of this work we will use \( E_{3\text{max}} = 14 \). Note that this truncation also works well for \(^{48}\text{Ca}\), as shown in the bottom part of Fig. 3.

![Graph](image)

**FIG. 3.** (Color online) Convergence of \( m_0 \) (a) and \( \alpha_D \) (b) calculated in the T-1/D scheme as a function of the number of configurations for the \( E_{3\text{max}} \). The adopted model space is \( N_{\text{max}} = 12 \). Each point corresponds to a jump of one unit (two units) in \( E_{3\text{max}} \) for \(^{48}\text{Ca} \) and selected values of \( E_{3\text{max}} \) are highlighted along the curves.

In Fig. 4 we show results for the \( m_0 \) sum rule (top) and the dipole polarizability (bottom) of \(^{16}\text{O}\) at \( \hbar \Omega = 22 \) MeV and \( E_{3\text{max}} = 14 \) as a function of \( N_{\text{max}} \). For \( m_0 \), the T-1/T-1 and T-1/D calculations almost coincide, while some difference is observed in \( \alpha_D \). The residual \( \hbar \Omega \) dependence amounts to about 1.5% in the largest model space. While in \(^{16}\text{O}\) the effect of triples is slightly larger than in \(^4\text{He}\), the overall effect of \( 3p-3h \) excitations is small and amounts to 4% and 6% for \( m_0 \) and \( \alpha_D \), respectively. Both for \( m_0 \) and \( \alpha_D \) the inclusion of \( 3p-3h \) excitations in the T-1/T-1 and T-1/D approaches reduce their magnitude as compared to the results obtained in the D/D approach.

![Graph](image)

**FIG. 4.** (Color online) Convergence of \( m_0 \) (a) and \( \alpha_D \) (b) for \(^{16}\text{O}\) with respect to the model-space size \( N_{\text{max}} \) for \( \hbar \Omega = 22 \) MeV and \( E_{3\text{max}} = 14 \). Two triples approximations schemes T-1/T-1 (green diamonds) and T-1/D (red circles) are compared to the D/D case (blue squares). The similarity transformed operator is implemented with Eq. (26) and (27) in T-1/T-1 and T-1/D, respectively.

In Fig. 5 we compare \( m_0 \) (a) and \( \alpha_D \) (b) for \(^{16}\text{O}\) obtained in the D/D (blue/right) scheme with the T-1/D (red/central) and the T-1/T-1 (green/right) approximations. The D/D value is obtained at \( N_{\text{max}} = 14 \) and \( \hbar \Omega = 22 \) MeV. Due to the large number of \( 3p-3h \) configurations, for \(^{16}\text{O}\) we are able to calculate only up to a maximum model space of \( N_{\text{max}} = 12 \) and \( E_{3\text{max}} = 14 \) for T-1/T-1. For consistent results we adopt the same truncation for \( E_{3\text{max}} \) in T-1/D. The bands in Fig. 5 are obtained by assigning a 2% uncertainty, accounting for the combined uncertainty from the \( E_{3\text{max}} \) cut and the residual \( \hbar \Omega \)-dependence.

Correlations arising from \( 3p-3h \) excitations reduce the size of these observables by a few percent, with effects being slightly larger on \( \alpha_D \) than for \( m_0 \). Similar to the \(^4\text{He}\) case, we find that results for \( m_0 \) obtained in the T-1/D and T-1/T-1 approaches almost coincide, while for \( \alpha_D \) they slightly differ. This is expected, because \( m_0 \)
is calculated as a ground-state expectation value, while $\alpha_D$ also requires the solution of the excited states from Eq. (10). We use the difference between the T-1/D and T-1/T-1 results as an estimate of neglected higher order correlations. This amounts to a 4% effect for $\alpha_D$ and an even smaller effect of 0.4% for $m_0$.

We now confront our results with data. Figure 5 compares the theoretical results with the experimental value obtained by integrating the data from Ahrens et al. [86] (grey bands). We see that the addition of triples leads to a deviation of $m_0$ and $\alpha_D$ with respect to the experimental data, which agreed better in the D/D approximation using the N$^2$LO$_{sat}$ interaction. We note that N$^2$LO$_{sat}$ was constrained to reproduce the charge radius of $^{16}$O using coupled-cluster theory in the D approximation. As shown in Refs. [12, 79], the charge radius is correlated with $\alpha_D$, and it would therefore be interesting to quantify the effect of $3p-3h$ excitations in the T-1 approach on charge radii as well. We also note that the extraction of these sum rules from photo-absorption data may be prone to larger systematic uncertainties than those quoted because it is not possible to estimate the role of multipoles beyond the dipole.

As the experimental determination of the dipole polarizability results from an integration of the dipole strength, it is interesting to study the running of the $\alpha_D$ sum rules as a function of the maximum integration limit. If one solves for the excited states in Eq. (10) using the Lanczos technique, it is possible to define the sum rule from the integral of the dipole response function $R(\omega)$ as

$$m_n(\varepsilon) = \int_0^\varepsilon d\omega \, \omega^n R(\omega),$$

and study its running as a function of $\varepsilon$. A discretized response function can also be obtained by a calculation of the Lorentz integral transform $I_L(\sigma, \Gamma)$ [57, 58] for a very small width parameter $\Gamma$ as (see Ref. [79] for details)

$$m_n(\varepsilon) = \lim_{\Gamma \to 0} \int_0^\varepsilon d\sigma \, \sigma^n I_L(\sigma, \Gamma).$$

The discretized response consists of smeared $\delta$ peaks and does not properly take the continuum into account. However, it will allow us to see how excited states and their corresponding strengths change within various approximation schemes, thus affecting the running sums.

The top of Fig. 6 shows the Lorentz integral transform calculated for $\Gamma = 0.01$ MeV (a) and running sum of $\alpha_D(\varepsilon)$ (b) for $^{16}$O with various coupled-cluster approximations compared with experimental results from Ahrens et al. [86].

![Figure 5: Comparison of $m_0$ (a) and $\alpha_D$ (b) in the D/D (blue/left), the T-1/D (red/central) and the T-1/T-1 (green/right) approximations against the integrated experimental data by Ahrens et al. in $^{16}$O.](image_1)

![Figure 6: Discretized response with $\Gamma = 0.01$ MeV (a) and running sum of $\alpha_D(\varepsilon)$ (b) for $^{16}$O with various coupled-cluster approximations compared with experimental results from Ahrens et al.](image_2)
TABLE III. Comparison of coupled-cluster results with self consistent Green’s function data from Ref. [30] in $^{48}$O using the N$^2$LO$_{sat}$ interaction.

<table>
<thead>
<tr>
<th>Method</th>
<th>$\alpha_D$ [fm$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ref. [30]</td>
<td>0.50</td>
</tr>
<tr>
<td>D/S</td>
<td>0.503</td>
</tr>
<tr>
<td>T-1/D</td>
<td>0.508</td>
</tr>
<tr>
<td>T-1/T-1</td>
<td>0.528</td>
</tr>
</tbody>
</table>

random phase approximation approach for the excited states. We find that the inclusion of $3p$-$3h$ correlations in the ground state and in the excited states decreases the polarizability with respect to a D/D calculation, making this more sophisticated calculation to coincidentally agree with simpler schemes, such as the D/S approximation.

IV. ELECTRIC DIPOLE POLARIZABILITY OF $^{48}$Ca

We now turn to our main goal and compute the dipole polarizability of $^{48}$Ca. In the recent experiment using proton inelastic scattering off a $^{48}$Ca target, the electric dipole strength was disentangled from other multipole contributions resulting in $\alpha_D = 2.07(22)$ fm$^3$ [1]. Overall, theory agreed with experiment, given the (still significant) systematic theoretical uncertainties as one varies the employed interaction. However, calculations based on interactions that reproduced the charge radius of $^{48}$Ca yielded results for $\alpha_D$ in the D/D approximation that were somewhat larger than the measured value. Those calculations were performed in the D/D approximation, and this makes it interesting to compute $\alpha_D$ with an increased precision by including leading-order $3p$-$3h$ correlations in the T-1 approximation.

Taking advantage of the results and benchmarks from Section III we revisit these calculations by using two established interactions, namely N$^2$LO$_{sat}$ and 1.8/2.0 (EM). These two interactions were also used in Refs. [4] [12]. The 1.8/2.0 (EM) potential is constructed following Ref. [57]. It starts from the chiral NN interaction at N$^2$LO [65] and “softens” it with the similarity renormalization group [47] at a cutoff/resolution scale $\lambda_{SRG} = 1.8$ fm$^{-1}$. The 3NF is taken as the leading chiral 3NF using a non-local regulator and cutoff $\lambda_{NF} = 2.0$ fm$^{-1}$, with short-ranged coefficients $c_D$ and $c_E$ adjusted to $A \leq 4$ nuclei. The “1.8/2.0 (EM)” interaction reproduces binding energies and spectra in medium-mass and heavy nuclei [30] [38], but yields too small charge radii. The N$^2$LO$_{sat}$ interaction yields radii in better agreement with data.

Figure 7 shows the $m_0$ sum rule (top) and the dipole polarizability $\alpha_D$ (bottom) obtained in the D/D and T-1/D approaches using the N$^2$LO$_{sat}$ (leftmost bands) and 1.8/2.0 (EM) (rightmost bands) interactions, respectively. The grey horizontal bands are data. For N$^2$LO$_{sat}$ we find that the addition of $3p$-$3h$ excitations in the ground state using the T-1 approach improves the agreement with the data. As calculations of excited states in the T-1 approach are computationally demanding and currently not feasible at sufficiently large $E_{\text{cut}}$, we did not employ the T-1/T-1 approach for $^{48}$Ca. However, based on our studies for $^4$He and $^{16}$O one may expect that the T-1/D and T-1/T-1 approaches would yield similar results.

We observe that both for $m_0$ and $\alpha_D$ the T-1 approximation for the ground state leads to a reduction of the strength, bringing theory in agreement with the recent data from Birkhan et al. [4]. Remarkably, the inclusion of leading triples corrections also reduces the Hamiltonian model dependence, leading to a more precise calculation of $m_0$ and $\alpha_D$. The effect of the triples on $\alpha_D$ amounts to 15% for the N$^2$LO$_{sat}$ and 6% for the 1.8/2.0 (EM) interaction, which is consistent with the latter being a much “softer” interaction. The triples effect on $m_0$ is smaller, amounting to about 5% for N$^2$LO$_{sat}$ and 2% for the 1.8/2.0 (EM) interaction. We also performed T-1 calculations for the charge radius of $^{48}$Ca, and found that inclusion of triples excitations increases the radius by about 1% for both the 1.8/2.0 (EM) and N$^2$LO$_{sat}$ interactions as compared to the D approximation. Thus, the effect of triples excitations on the charge radius of $^{48}$Ca is negligible, and the results and conclusions of Ref. [48] are accurate.
FIG. 8. (Color online) Discretized response with $\Gamma = 0.01$ MeV (a) and running sum of $\alpha_D(\varepsilon)$ (b) for $^{48}$Ca with various coupled-cluster approximations compared with experimental results from Birkhan et al. [4].

Interestingly, for $^{48}$Ca we see that for the D/S approximation the strength is dominated by a single state at around 19 MeV of excitation energy, while higher-order correlations included in D/D and T-1/D shift and fragment the strength significantly. The inclusion of 3p-3h excitations via the T-1 approach in the ground state, makes the strength more fragmented and also increases some of the strength at higher energy. Such fragmentation combined with the inverse energy weight in the polarizability sum rule is the mechanisms that leads to a reduction of $\alpha_D$. Opposite to what was found in $^{16}$O, for $^{48}$Ca the computationally least expensive D/S approximation coincidentally agrees with D/D and not with the computationally most expensive approximation (T-1/D in this case).

V. CONCLUSIONS

We computed the electric dipole polarizability $\alpha_D$ of $^{48}$Ca with an increased precision by including leading 3p-3h correlations. Leading order 3p-3h excitations were implemented in the CCSDT-1 approximation for the ground state, excited states, and the similarity transformed dipole operator. The effect of 3p-3h excitations on the latter was found to be negligible. The inclusion of 3p-3h excitations in the ground state via CCSDT-1 is sufficient to obtain an agreement with the hyperspherical harmonics approach for $^{4}$He to better than 1%. While the effect of triples is quite small in $^{4}$He, it becomes larger in $^{16}$O and $^{48}$Ca. In $^{16}$O triples excitations reduce the size of $m_0$ sum rule and $\alpha_D$ by about 4-6%. In $^{48}$Ca they reduce $\alpha_D$ by about a 15% reduction for the N$^2$LO$_{sat}$ interaction and by about 6% for the 1.8/2.0 (EM) interaction. This brings our coupled-cluster calculations in agreement with the recent experimental result obtained from inelastic proton scattering [4]. The effect of triples excitations is smaller for the $m_0$ sum rule in $^{48}$Ca, and reduces it by about 5% and 2% for the two interactions considered, respectively. Finally we found that the effect of triples excitations on the charge radius of $^{48}$Ca is negligible, and increases it by about 1% for both interactions considered in this work.

We note that some simpler approximations may occasionally coincide with more sophisticated computations using the CCSDT-1 method both for the ground and excited states. We conclude that the effect of 3p-3h excitations in the ground state is more important than their effect in excited states for the electromagnetic sum rules studied in this work. The inclusion of triples excitations in the excited states, while possible for light nuclei such as $^{4}$He and $^{16}$O, will require further developments in order to overcome the hurdles associated with the increase in computational cost for heavier nuclei. We expect our results also to be relevant for other many-body approaches, such as the self consistent Green’s function and the in medium similarity renormalization group methods.

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