

## Coulomb sum rule for ${}^4\text{He}$ and ${}^{16}\text{O}$ from coupled-cluster theory

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We demonstrate the capability of coupled-cluster theory to compute the Coulomb sum rule for the  ${}^4\text{He}$  and  ${}^{16}\text{O}$  nuclei using interactions from chiral effective field theory. We perform several checks, including a few-body benchmark for  ${}^4\text{He}$ . We provide an analysis of the center-of-mass contaminations, which we are able to safely remove. We then compare with other theoretical results and experimental data available in the literature, obtaining a fair agreement. This is a first and necessary step towards initiating a program for computing neutrino-nucleus interactions from first principles in coupled-cluster theory and supporting the experimental long-baseline neutrino program with a state-of-the-art theory that can reach medium-mass nuclei.

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### I. INTRODUCTION

Current neutrino oscillation experiments such as Mini-BooNE [1] and T2K [2] as well as future experiments such as DUNE [3] and T2HK [4] are entering a precision phase, with an uncertainty goal of the order of a percent. Accurate extraction of neutrino oscillation parameters from these experiments requires a reliable theoretical treatment of the scattering of neutrinos with nuclei that constitute the detector material. Presently, the analysis of data is systematically affected by crude nuclear physics models. Based on existing studies, nuclear structure uncertainties are estimated to be of the order of ten percent [5]. A comprehensive understanding of interactions of neutrinos with nuclei, built on a cutting edge theory with the capability of reliably estimating uncertainties, is urgently needed. Since the energy spectrum of the neutrinos typically ranges from the MeV to the GeV scale, different mechanisms are at play: quasielastic scattering,  $\Delta$  and  $\pi$  production, and deep inelastic scattering. The quasielastic process, which dominates the scattering at sub-GeV energies, makes a significant contribution to the total cross section and is the dominant process in the T2HK experiment, in which the neutrino beam peaks at energies of the order of 600 MeV. The quasielastic scattering regime is amenable to *ab initio* treatment of nuclei in terms of constituent neutrons and protons, with nuclear interaction and electroweak currents grounded in chiral effective field theory ( $\chi$ EFT). At present, this approach offers the best opportunity for a direct connection to quantum chromodynamics and a solid uncertainty quantification.

*Ab initio* calculations of neutrino interactions on medium-mass nuclei with modern nuclear interactions have so far been performed using the Green's function Monte Carlo method [6–8] and the self-consistent Green's function method [9]. By combining the Lorentz integral transform (LIT) [10,11] with coupled-cluster (CC) theory [12] and merging them

into a method called LIT-CC, we plan to develop a new *ab initio* approach to compute general electroweak responses in medium-mass nuclei. This paper marks a significant milestone in this direction. We build upon the progress made in investigating the electron-scattering reactions of light nuclei within the LIT method (see, e.g., Refs. [13–15]) and the studies of the giant dipole resonances of light and medium-mass nuclei using the LIT-CC approach [16,17]. Here, we calculate the Coulomb sum rule (CSR) for  ${}^4\text{He}$  and  ${}^{16}\text{O}$  from coupled-cluster theory. While calculations of the CSR for  ${}^{16}\text{O}$  from coupled-cluster theory already exist in the literature [18], we present a different approach with a clear goal of extending the LIT-CC formalism to neutrino scattering in the future. We identify, understand, and tackle a problem in the LIT-CC method which is relevant for lepton-nucleus scattering: translationally noninvariant operators induce excitations of the nuclear center-of-mass (CoM) wave function which leads to spuriousities in the calculations of electroweak responses and sum rules. We show that this CoM contamination in the CSR can be removed to a very good approximation by projecting the final states in the matrix elements out of the subspace spanned by states with CoM excitations.

The paper is organized as follows. In Sec. II we present some general formulas for the Coulomb sum rule. Sec. III contains a brief introduction to coupled-cluster theory. We present several benchmarks in Sec. IV, show an analysis of the spurious center-of-mass states in Sec. V, and provide a comparison with other available calculations and experimental data in Sec. VI. Finally, in Sec. VII, we present a brief summary and outlook.

### II. THE COULOMB SUM RULE

The electromagnetic sum rules have provided stringent tests for theories and experiments on electro- and

photonuclear scattering since the early years of quantum mechanics. The CSR, in particular, has played a major role in building our understanding of nuclear physics beyond a simple model of the nucleus as a collection of non-relativistic pointlike protons and neutrons bound by a mean field [19]. It continues to guide the development of theories for nuclear electroweak processes (see, e.g., Ref. [20]) because it allows us to study the response of the nucleus to an external probe induced by the charge operator with the nuclear excitation spectrum integrated out. Formally, the CSR can be defined as an inelastic sum rule [19] as

$$\begin{aligned} m_0^{\text{in}}(q) &= \sum_{f_1}^{\infty} |\langle f_1 | \rho_1(q) | 0_1 \rangle|^2 - |\langle 0_1 | \rho_1(q) | 0_1 \rangle|^2, \\ &= m_0(q) - Z^2 |F_{\text{el}}(q)|^2, \end{aligned} \quad (1)$$

where the first term on the right-hand side is the total sum rule of order 0, itself defined as

$$m_0(q) = \sum_{f_1}^{\infty} |\langle f_1 | \rho_1(q) | 0_1 \rangle|^2 = \langle 0_1 | \rho_1^\dagger(q) \rho_1(q) | 0_1 \rangle, \quad (2)$$

and the term  $|F_{\text{el}}(q)|^2 = |\langle 0_1 | \rho_1(q) | 0_1 \rangle|^2 / Z^2$  is the square of the elastic charge form factor of the nucleus. The state  $|0_1\rangle$  is the intrinsic ground state of the nucleus and  $|f_1\rangle$  runs over a complete set of states.

If we consider pointlike nucleons and choose the direction of the transfer momentum  $\mathbf{q}$  along the  $z$  axis, the charge operator can be written in the intrinsic frame as

$$\rho_1(q) = \sum_{j=1}^Z e^{iqz'_j}, \quad (3)$$

where  $z'_j = z_j - Z_{\text{CoM}}$  are the particle coordinates ( $z$  components) relative to the CoM. In the laboratory system, however, the charge operator is

$$\rho(q) = \sum_{j=1}^Z e^{iqz_j}, \quad (4)$$

where  $z_j$  are the laboratory coordinates, as used in coupled-cluster theory.

### A. CSR as a ground state expectation value

The charge operator written in the laboratory frame factorizes into the product of an intrinsic operator and a CoM operator since

$$\rho(q) = \sum_{j=1}^Z e^{iqz'_j} e^{iqZ_{\text{CoM}}} = \rho_1(q) e^{iqZ_{\text{CoM}}}. \quad (5)$$

As a consequence, we have translational invariance for

$$\rho_1^\dagger(q) \rho_1(q) = \rho^\dagger(q) \rho(q), \quad (6)$$

at the operatorial level. Furthermore, assuming an exact factorization of the ground state wave functions into intrinsic and

CoM part as

$$|0\rangle = |0_1\rangle |0_{\text{CoM}}\rangle, \quad (7)$$

we can formally show that a calculation of  $m_0(q)$  in the laboratory frame directly yields the intrinsic-frame result:

$$\begin{aligned} \langle 0 | \rho^\dagger(q) \rho(q) | 0 \rangle &= \langle 0_1 | \rho_1^\dagger(q) \rho_1(q) | 0_1 \rangle \langle 0_{\text{CoM}} | 0_{\text{CoM}} \rangle \\ &= \langle 0_1 | \rho_1^\dagger(q) \rho_1(q) | 0_1 \rangle = m_0(q). \end{aligned} \quad (8)$$

Calculating  $m_0(q)$  in this manner as the ground state expectation value of the two-body operator  $\rho^\dagger(q) \rho(q)$  reveals that it is related to the Fourier transform of the proton-proton distribution function

$$f_{pp}(q) = \frac{1}{Z(Z-1)} \langle 0_1 | \sum_{j \neq k}^Z e^{-iq(z_k - z_j)} | 0_1 \rangle \quad (9)$$

by [19]

$$m_0(q) = Z + Z(Z-1) f_{pp}(q). \quad (10)$$

To obtain the Coulomb sum rule from  $m_0(q)$  as in Eq. (1), we need to subtract the elastic part by calculating the form factor. In coupled-cluster theory, the form factor is first obtained in the laboratory frame as

$$|F(q)|^2 = \frac{1}{Z^2} |\langle 0 | \rho(q) | 0 \rangle|^2. \quad (11)$$

Assuming again the separable ansatz of the ground state as shown in Eq. (7) and using the factorization of the charge operator from Eq. (5), this becomes

$$\begin{aligned} |F(q)|^2 &= \frac{1}{Z^2} |\langle 0_1 | \rho_1(q) | 0_1 \rangle|^2 |\langle 0_{\text{CoM}} | e^{iqZ_{\text{CoM}}} | 0_{\text{CoM}} \rangle|^2 \\ &= |F_{\text{el}}(q)|^2 |\langle 0_{\text{CoM}} | e^{iqZ_{\text{CoM}}} | 0_{\text{CoM}} \rangle|^2. \end{aligned} \quad (12)$$

As demonstrated in Refs. [21–23], the wave-function factorization in Eq. (7) is valid to a high precision in coupled-cluster theory. Furthermore,  $|0_{\text{CoM}}\rangle$  is the ground state of a harmonic oscillator with a fixed frequency  $\tilde{\omega}$  that can be determined by requiring that the coupled-cluster ground state expectation value of the CoM Hamiltonian,  $P_{\text{CoM}}^2/(2M) + 1/2M\tilde{\omega}^2 R_{\text{CoM}}^2 - 3/2\hbar\tilde{\omega}$ , vanishes. One can therefore easily calculate  $|\langle 0_{\text{CoM}} | e^{iqZ_{\text{CoM}}} | 0_{\text{CoM}} \rangle|^2$ .  $|F_{\text{el}}(q)|^2$  thus obtained from Eqs. (11) and (12) is then subtracted from  $m_0(q)$  given by Eq. (8), yielding the Coulomb sum rule  $m_0^{\text{in}}(q)$ . Calculating the CSR in this manner is denoted as “method A” in the rest of the paper. We expect this approach to be free of contaminations from the CoM wave function to a good level of approximation. For  ${}^4\text{He}$ , we will numerically verify this by comparing calculations performed in the laboratory frame using coupled-cluster theory with calculations obtained from hyperspherical harmonics working in the intrinsic frame.

### B. CSR as sum over multipoles

The approach of Sec. II A is not applicable in general to the calculation of sum rules and response functions of the large set of electroweak charge and current operators we will need to include in neutrino scattering calculations. The standard approach while working with angular momentum eigenstates is to perform a multipole decomposition of the electroweak

operators; see, e.g., Ref. [24]. We therefore expand the charge operator into multipoles as

$$\rho(q) = \sum_{J=0}^{\infty} [\rho(q)]^J. \quad (13)$$

In practice, the infinite sum over  $J$  needs to be truncated at a finite multipolarity. The number of multipoles needed to achieve convergence depends on the momentum  $q$  and the size of the nucleus. We obtain  $m_0(q)$  as a coherent sum,

$$m_0(q) = \sum_{J=0}^{\infty} m_0^J(q), \quad (14)$$

where

$$\begin{aligned} m_0^J(q) &= \langle 0 | [\rho^\dagger(q)]^J [\rho(q)]^J | 0 \rangle \\ &= \sum_{f^J} \langle 0 | [\rho^\dagger(q)]^J | f^J \rangle \langle f^J | [\rho(q)]^J | 0 \rangle. \end{aligned} \quad (15)$$

is the total strength of each multipole operator. Here we have inserted the completeness relation in terms of states  $|f^J\rangle$  labeled by total angular momentum quantum number  $J$ , only retained nonvanishing terms, and have restricted ourselves to the case where the nuclear ground state  $|0\rangle$  has zero total angular momentum. The elastic part can be subtracted by simply restricting the sum over  $f^J$  to  $|f^J\rangle \neq |0\rangle$  in Eq. (15). In this way we remove the contribution coming from the laboratory form factor  $|F(q)|^2$ , which is not the same as the removal of  $|F_{\text{el}}(q)|^2$  in method A.

At this point it is important to note that, since the operator  $[\rho(q)]^J$  is not translationally invariant, the states  $|f^J\rangle$  can contain CoM excitations. Translationally noninvariant operators can generate CoM excitations by acting on  $|0_{\text{CoM}}\rangle$  even if the ground state  $|0\rangle$  factorizes exactly as shown in Eq. (7). We expect such spurious excitations to make significant contributions to the sum rule for the lowest multipoles. In Sec. V, we will discuss how we remove these CoM excitations and demonstrate it with a practical numerical implementation. Let us note that spurious CoM contamination could also be present when using translationally invariant operators such as the electric dipole [17] if the factorization shown in Eq. (7) is inexact. In the LIT-CC method, they can be removed in the Lanczos algorithm, as done in Ref. [17]. In this work we will use a similar technique (described below), and calculating the CSR in this way will be called “method B” in the rest of the paper.

### III. COUPLED-CLUSTER THEORY

In coupled-cluster theory [18,23,25–31] one uses the similarity transformed Hamiltonian,

$$\bar{H}_N = e^{-T} H_N e^T, \quad T = T_1 + T_2 + \dots, \quad (16)$$

where  $H_N$  is normal ordered with respect to a single reference state  $|\Phi_0\rangle$  (usually a Slater determinant obtained from a Hartree-Fock calculation), and  $T$  is an expansion in particle-hole excitations with respect to this reference. The operator  $T$  is typically truncated at some low rank particle-hole excitation level.

Because the similarity transformed Hamiltonian is non-Hermitian, one has to compute both the left and right eigenstates in order to evaluate expectation values and transition strengths. The right ground state is  $|0\rangle = |\Phi_0\rangle$  while left ground state is obtained as

$$\langle 0 | = \langle \Phi_0 | (1 + \Lambda), \quad \Lambda = \Lambda_1 + \Lambda_2 + \dots, \quad (17)$$

where  $\Lambda$  is a sum of particle-hole deexcitation operators.

In the LIT-CC method, we use the coupled-cluster equation-of-motion (EOM) method [23,32] together with a nonsymmetric Lanczos algorithm to solve for a generalized non-Hermitian eigenvalue problem with a source term (see Ref. [33] for details). In practice one deals with the excited states of the Hamiltonian defined as

$$\begin{aligned} \bar{H}_N R_\mu |\Phi_0\rangle &= E_\mu R_\mu |\Phi_0\rangle, \\ \langle \Phi_0 | L_\mu \bar{H}_N &= E_\mu \langle \Phi_0 | L_\mu, \end{aligned} \quad (18)$$

where  $R_\mu$  and  $L_\mu$  are linear expansions in particle-hole excitations as well. To compute an electromagnetic transition strength from the ground to an excited state in coupled-cluster theory, one performs the following calculation (see Ref. [33]):

$$\begin{aligned} |\langle f_\mu | \hat{\Theta} | 0 \rangle|^2 &= \langle 0 | \hat{\Theta}^\dagger | f_\mu \rangle \langle f_\mu | \hat{\Theta} | 0 \rangle \\ &= \langle \Phi_0 | (1 + \Lambda) \bar{\Theta}_N^\dagger R_\mu | \Phi_0 \rangle \langle \Phi_0 | L_\mu \bar{\Theta}_N | \Phi_0 \rangle, \end{aligned} \quad (19)$$

where  $\bar{\Theta}_N \equiv e^{-T} \Theta_N e^T$  is the similarity transformed normal-ordered operator. In this work the operator is taken to be an electromagnetic Coulomb multipole of rank  $J$ , namely  $\Theta = [\rho(q)]^J$  (see also Ref. [24]), and a summation on the multipoles is performed afterwards. The Coulomb multipoles are one-body operators, so that the Baker-Campbell-Hausdorff expansion for  $\bar{\Theta}_N$  terminates at doubly nested commutators

$$\bar{\Theta}_N = \Theta_N + [\Theta_N, T] + \frac{1}{2} [[\Theta_N, T], T]. \quad (20)$$

Finally, the total multipole strength as calculated in method B is [33]

$$m_0^J(q) = \langle v_L^J | v_R^J \rangle = \langle \Phi_0 | (1 + \Lambda) \bar{\Theta}_N^\dagger \cdot \bar{\Theta}_N | \Phi_0 \rangle, \quad (21)$$

where we used the closure relation. Let us label the spurious excitations of angular momentum  $J$  by  $s^J$ . The spurious states as well as the ground state are obtained from the coupled-cluster EOM technique using an iterative Arnoldi algorithm. Having obtained the converged left  $\langle s_L^J |$  and right  $|s_R^J\rangle$  spurious states, we project them out of Eq. (21) by multiplying the left  $\langle v_L^J |$  and right  $|v_R^J\rangle$  states with  $(\mathbf{1} - |s_R^J\rangle \langle s_L^J|)$  to obtain

$$\bar{m}_0^J(q) = \langle v_L^J | v_R^J \rangle - \langle v_L^J | s_R^J \rangle \langle s_L^J | v_R^J \rangle \quad (22)$$

(see Sec. V below for further details).

In both methods A and B, the computation of the CSR is performed in the so-called coupled-cluster with singles-and-doubles (CCSD) approximation, where all the particle-hole expansions mentioned above are truncated at the two-particle-two-hole level. While we have developed the necessary technology to deal with leading-order triple corrections, in Ref. [33] we found that they are negligible for non-energy-weighted sum rules (as the CSR is); furthermore these excitations increase the computational cost by about an order

of magnitude. Hence, we neglect them at this point and focus on studying the momentum dependence of our results.

#### IV. BENCHMARKS

We employ Hamiltonians from  $\chi$ EFT in our calculations. Specifically, we employ two interactions. First, we use the nucleon-nucleon ( $NN$ ) chiral potential by Entem and Machleidt [34] (labeled by  $N^3$ LO-EM) without supplementing it with a three-nucleon ( $3N$ ) interaction. This will serve to perform tests with hyperspherical harmonics expansion [35] in  ${}^4\text{He}$  and to perform an analysis of the center-of-mass spuriousities. Second, we use the  $\text{NNLO}_{\text{sat}}$  interaction [36], that includes both  $NN$  and  $3N$  interactions at next-to-next-to leading order in  $\chi$ EFT. In this case, the parameters entering the  $NN$  and  $3N$  interactions were adjusted to  $NN$  phase shifts and to energies and charge radii of selected nuclei up to  ${}^{24}\text{O}$ . We use this interaction because it has been shown to work well for the nuclei studied in this paper.

*Few-body benchmark for  ${}^4\text{He}$ .* We start by presenting our results from coupled-cluster theory obtained from method A using the  $N^3$ LO-EM  $NN$  interaction. In Fig. 1, we show separately the elastic squared form factor  $|F_{\text{el}}(q)|^2$  and the proton-proton distribution function  $f_{pp}(q)$ , that are related to CSR by Eqs. (1) and (10). The calculations is performed in the CCSD scheme for a model space of 15 major oscillator shells and an underlying harmonic oscillator frequency of  $\hbar\omega = 20$  MeV. In order to remove the CoM contamination from  $|F_{\text{el}}(q)|^2$  [see Eq. (12)], an underlying CoM frequency  $\hbar\tilde{\omega} = 20$  MeV was employed, which is known from Ref. [21]. We compare it to calculations performed with the hyperspherical harmonics method (HH) [37] using the same potential. Such few-body computations have been performed with a model space of  $K_{\text{max}} = 16$  in the HH method, where the accuracy is expected to be of about a percent. As one can see, the agreement is very good over a wide range of momentum transfer  $q$ , indicating that for the  ${}^4\text{He}$  and chiral potentials triples and quadrupole excitations missing in the CCSD approximation can safely be neglected. Only for the function  $f_{pp}(q)$ , one can see a deviation of the two curves at the largest shown momenta. However, since this quantity is much smaller than 1 at high  $q$  values, the observed alignment of the HH and CCSD curves leads to a nice agreement at the CSR level. This allows us to infer that the factorization of the wave function into a CoM and an intrinsic part must hold to a large extent, since a calculation performed in the laboratory frame agrees with the one in the intrinsic frame.

*Comparison of two calculational methods.* At this point, we proceed with tests of the coupled-cluster computations, namely we want to verify if methods A and B agree with each other. As mentioned above, method B may include spurious states that need to be removed. Because identifying all spurious states by running the full protocol described in Refs. [22,38] is computationally demanding, we adopt a more pragmatic strategy in this work. For  ${}^4\text{He}$ , we omit from the Lanczos iterations all states with excitation energy below 15/MeV, as they have to be spurious given that  ${}^4\text{He}$  has no

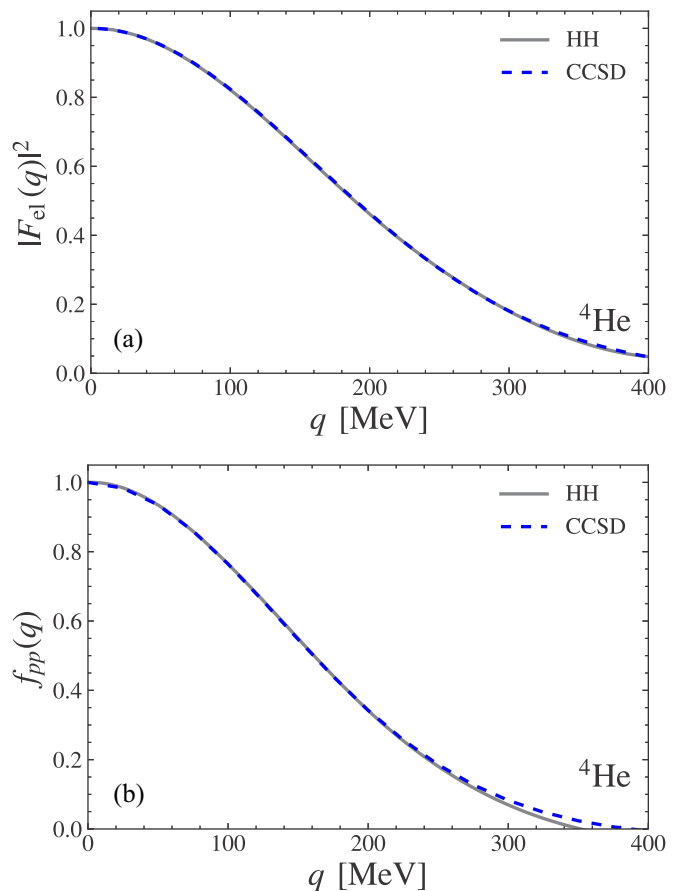


FIG. 1. Coupled-cluster calculations in CCSD compared against HH using the  $N^3$ LO-EM interaction. The two separate components making up the CSR, namely the squared elastic form factor  $|F_{\text{el}}(q)|^2$  (a) and  $f_{pp}(q)$  (b) are shown as functions of the momentum transfer  $q$ .

excited state below the proton emission threshold. For the chosen interaction and model space, the omitted states were a  $1^-$  state approximately at energy  $5 \times 10^{-2}$  MeV above the ground state and a  $2^+$  state at energy 10 MeV above the ground state. For  ${}^{16}\text{O}$ , we remove a  $1^-$  state at 0.15 MeV, which also must be spurious as this nucleus does not have any excited states at such low energy.

In Fig. 2 we show a comparison between method A and method B for  ${}^4\text{He}$  and  ${}^{16}\text{O}$  using the  $N^3$ LO-EM interaction. For method B we show the curve obtained in the case where we do not remove the spurious states in the Lanczos procedure as well as the one where we remove such states. Calculations are performed for a model space of 15 oscillator shells and a harmonic oscillator frequency of  $\hbar\omega = 20$  MeV for all the three curves. In case of  ${}^{16}\text{O}$  we show a band obtained by the difference between the model spaces with 15 and 13 major shells. This gives us an idea of the uncertainty in a model space size that will be achievable in other calculations where we will add  $3N$  interactions.

First of all, we see that the removal of the spuriousities has a much larger effect in  ${}^4\text{He}$  than in  ${}^{16}\text{O}$ , as expected, since the heavier the nucleus, the smaller the CoM contamination

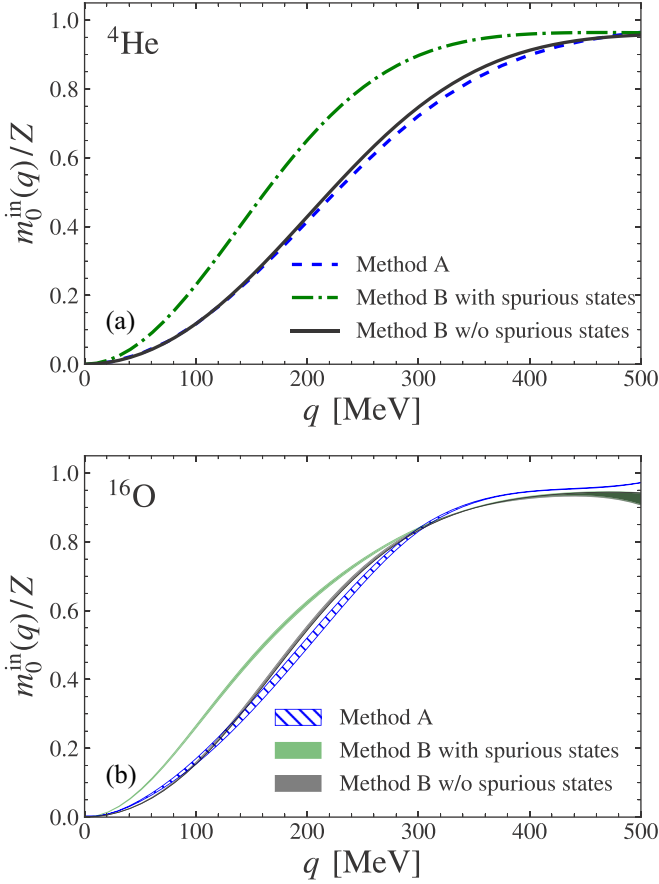


FIG. 2. Comparison of methods A and B: for  ${}^4\text{He}$  (a) and  ${}^{16}\text{O}$  (b) using the  $\text{N}^3\text{LO-EM}$  interaction. For method B we show the cases with and without (w/o) spurious CoM states.

must be. Second, we see that the results of method B without spurious states agree quite nicely with those of method A for both nuclei. The removal of spurious states brings the agreement at  $q = 100$  MeV from 50% (38%) to 0.5% (3.5%) for  ${}^4\text{He}$  ( ${}^{16}\text{O}$ ), while at  $q = 200$  MeV it brings the agreement from 35% (20%) to 3% (8%). We consider this comparison satisfactory and from now on we will use method B only without the spurious states to perform further analysis.

*Convergence of multipole expansion.* A natural question in method B is how many multipoles are needed in the expansion of Eq. (3). We show this for the  $\text{N}^3\text{LO-EM}$   $NN$  interaction in Fig. 3. These calculations are performed for the same model space as above. Clearly, the convergence in terms of multipoles strongly depends on the momentum transfer, as expected. Furthermore, we see that the convergence is faster for the smaller  ${}^4\text{He}$  nucleus than for the larger  ${}^{16}\text{O}$  nucleus. For  $q$  below 200 MeV only four multipoles are needed, while for  $q = 500$  MeV nine and eleven multipoles are needed to reach satisfactory convergence for  ${}^4\text{He}$  and  ${}^{16}\text{O}$ , respectively. The information on the number of needed multipoles will be relevant to estimate the amount of computing time requested to compute response functions with the LIT-CC method. Otherwise, the CSR can be most efficiently computed with method A instead.

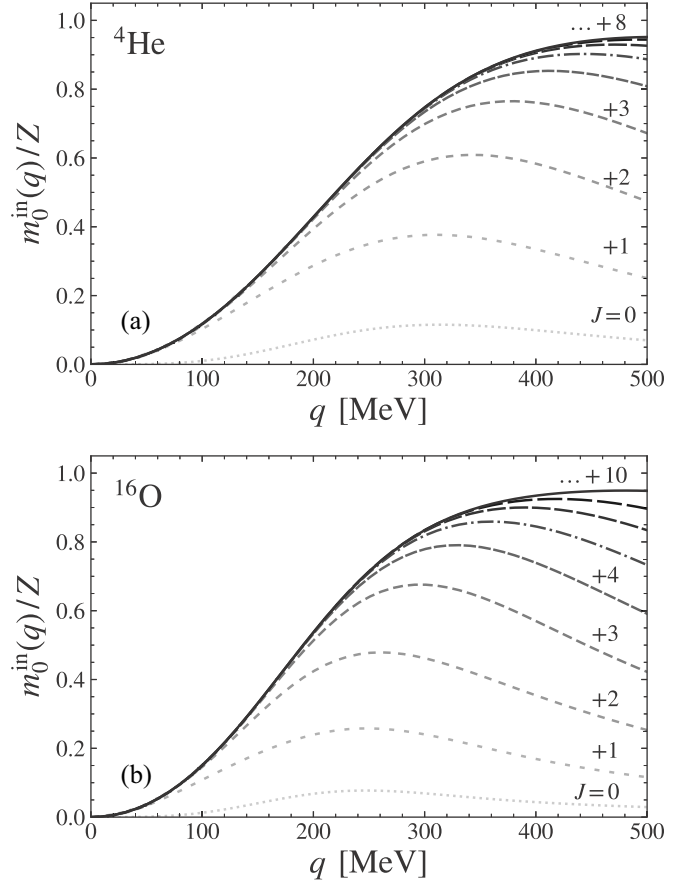


FIG. 3. Cumulative sums of the multipole expansion for the Coulomb sum rule of  ${}^4\text{He}$  (a) and  ${}^{16}\text{O}$  (b) using the  $\text{N}^3\text{LO-EM}$  interaction in method B w/o spurious states.

## V. ANALYSIS OF SPURIOUS STATES

In method B we find that by far the largest spurious contribution that we remove comes from the  $1^-$  state. In order to understand the nature of the spurious states we removed, let us assume for the moment that the factorization of  $|0\rangle$  into  $|0_I\rangle|0_{\text{CoM}}\rangle$  is exact, with  $|0_{\text{CoM}}\rangle$  being the ground state of a quantum harmonic oscillator. The nonspurious excitations are those that have the form  $|f_I^J\rangle|0_{\text{CoM}}\rangle$ , where  $|f_I^J\rangle$  are excitations of the intrinsic wave function, labeled by total angular momentum quantum number  $J$ . The simplest possible form of the spurious states is then  $|0_I\rangle|f_{\text{CoM}}^J\rangle$ , where  $|f_{\text{CoM}}^J\rangle$  are excitations of the CoM wave function. The completeness relation used in Eq. (15) then separates into the projectors onto the coupled-cluster ground state, the subspace spanned by nonspurious excitations, and the subspace spanned by spurious excitations, as

$$\begin{aligned} \sum_{f^J} |f^J\rangle\langle f^J| &\simeq |0_I\rangle|0_{\text{CoM}}\rangle\langle 0_{\text{CoM}}|\langle 0_I| \\ &+ \sum_{f_I^J} |f_I^J\rangle|0_{\text{CoM}}\rangle\langle 0_{\text{CoM}}|\langle f_I^J| \\ &+ \sum_{f_{\text{CoM}}^J} |0_I\rangle|f_{\text{CoM}}^J\rangle\langle f_{\text{CoM}}^J|\langle 0_I|. \end{aligned} \quad (23)$$

Inserting this relation in Eq. (15), we obtain

$$m_0^J(q) = Z^2 |F(q)|^2 \delta_{J0} + [m_0^{\text{in}}(q)]^J + [m_0^{\text{sp}}(q)]^J, \quad (24)$$

where the first term on the right-hand side is the squared elastic form factor in the laboratory frame and only contributes to the monopole term, the second term is the multipole strength of the CSR and the third term is the contribution of the spurious states to  $m_0^J(q)$ .

The Coulomb sum rule,

$$m_0^{\text{in}}(q) = \sum_{J=0}^{\infty} [m_0^{\text{in}}(q)]^J, \quad (25)$$

which is calculated in practice by adding a finite number of multipoles until convergence is achieved, is then free of contributions from CoM excitations. The spurious state contribution  $[m_0^{\text{sp}}(q)]^J$  is given by the squared matrix element:

$$\begin{aligned} [m_0^{\text{sp}}(q)]^J &= |\langle 0_{\text{I}} | \langle f_{\text{CoM}}^J | [\rho' ]_0^J | 0 \rangle|^2 \\ &= |\langle 0_{\text{I}} | \langle f_{\text{CoM}}^J | [[\rho' ]_{m_1}^{J_1} \otimes [e^{iqZ_{\text{CoM}}}]_{m_2}^{J_2}]_0^J | 0_{\text{I}} \rangle | 0_{\text{CoM}} \rangle|^2 \\ &= \left| \sum_m C_{00J0}^{J_1 J_2} \langle 0_{\text{I}} | [\rho' ]_0^J | 0_{\text{I}} \rangle \langle f_{\text{CoM}}^J | [e^{iqZ_{\text{CoM}}}]_0^J | 0_{\text{CoM}} \rangle \right|^2 \\ &= Z^2 |F_{\text{el}}(q)|^2 K_{\text{CoM}}^J(q), \end{aligned} \quad (26)$$

where  $C_{J_1 m_1 J_2 m_2}^{J m}$  are Clebsch-Gordan coefficients and

$$K_{\text{CoM}}^J(q) = |\langle f_{\text{CoM}}^J | [e^{iqZ_{\text{CoM}}}]_0^J | 0_{\text{CoM}} \rangle|^2 \quad (27)$$

depend only on the CoM.

It was shown in Ref. [21] that the CoM part of the coupled-cluster ground state,  $|0_{\text{CoM}}\rangle$ , is well approximated by the ground state of a three-dimensional harmonic oscillator Hamiltonian with energy eigenvalues  $E = \hbar\tilde{\omega}(N + \frac{3}{2})$ , where the number of oscillator quanta  $N$  is related to the radial quantum number  $N_r$  and the angular momentum quantum number  $J$  by  $N = 2N_r + J$  with  $J \leq N$ . The oscillator length parameter is  $b = \sqrt{\frac{\hbar}{2M\tilde{\omega}}}$ , where  $M$  is the mass of the nucleus.

Here, we make the ansatz that the CoM part of the spurious state,  $|f_{\text{CoM}}^J\rangle$ , is given by the excited oscillator state  $|\Psi_{0J0}^{\text{CoM}}\rangle$ . The CoM functions  $K_{\text{CoM}}^J(q)$  can then be written as

$$K_{\text{CoM}}^J(q) = |\langle \Psi_{0J0}^{\text{CoM}} | [e^{iqZ_{\text{CoM}}}]_0^J | \Psi_{000}^{\text{CoM}} \rangle|^2, \quad (28)$$

and calculated using coordinate representations of the oscillator states,

$$\begin{aligned} \langle \mathbf{R}_{\text{CoM}} | \Psi_{N_r J M}^{\text{CoM}} \rangle &= \sqrt{\frac{2N_r!}{b^3 \Gamma(N_r + J + 3/2)}} \left( \frac{R_{\text{CoM}}}{b} \right)^J \\ &\times \exp\left(-\frac{R_{\text{CoM}}^2}{2b^2}\right) L_{N_r}^{J+\frac{1}{2}}\left(\frac{R_{\text{CoM}}^2}{b^2}\right) \\ &\times Y_{JM}(\hat{\mathbf{R}}_{\text{CoM}}), \end{aligned} \quad (29)$$

where  $L_n^\ell(x)$  are associated Laguerre polynomials which satisfy  $L_0^\ell(x) = 1$  for all values of  $\ell$  and  $x$ . This yields

$$K_{\text{CoM}}^J(q) = \frac{\sqrt{\pi}(2J+1)}{2\Gamma(J+3/2)} \left(\frac{bq}{2}\right)^{2J} \exp\left(-\frac{b^2 q^2}{2}\right). \quad (30)$$

A closed-form expression for  $K_{\text{CoM}}^J(q)$  can also be obtained for a more general ansatz,  $|f_{\text{CoM}}^J\rangle = |\Psi_{N_r J 0}^{\text{CoM}}\rangle$ , which allows the spurious states to contain radial excitations with  $N_r > 0$ . This derivation, along with a detailed numerical analysis of such excitations, will be communicated through a separate publication [39]. However, we do find that radial excitations are negligible in the following analysis, hence we keep our ansatz as simple as possible.

Let  $\bar{m}_0^J(q)$  be the multipole strength calculated by removing a spurious state of angular momentum  $J$  (and the ground state for  $J = 0$ ) in the Lanczos procedure, defined in Eq. (22). The difference  $m_0^J(q) - \bar{m}_0^J(q)$  can then be obtained in the LIT-CC method, which allows us to numerically check whether

$$m_0^J(q) - \bar{m}_0^J(q) = Z^2 |F_{\text{el}}(q)|^2 K_{\text{CoM}}^J(q) \quad (31)$$

holds for the expression for  $K_{\text{CoM}}^J(q)$  given by Eq. (30). We thus validate all our assumptions about the nature of the CoM spuriousity.

It is important to realize, that summing Eq. (31) over  $J$ , we obtain<sup>1</sup>

$$m_0(q) - \bar{m}_0(q) = Z^2 |F_{\text{el}}(q)|^2 \sum_{J=0}^{\infty} K_{\text{CoM}}^J(q) \approx Z^2 |F_{\text{el}}(q)|^2. \quad (32)$$

On the left-hand side we have the sum of all the spurious states (with the ground state in the laboratory frame included) obtained numerically. It should correspond to the elastic form factor squared, so one can see here a direct connection with Eq. (1).

Let us note that, for  $J = 0$ , we have that  $K_{\text{CoM}}^0(q) = |\langle 0_{\text{CoM}} | e^{iqZ_{\text{CoM}}} | 0_{\text{CoM}} \rangle|^2$ , and so in Eq. (31) on the right-hand side we obtain  $Z^2 |F(q)|^2$  which stays in agreement with Eq. (12). This way we show that Eq. (31) holds for  $J = 0$ .

In Fig. 4, we plot the contributions of the  $1^-$  spurious states to the sum rules for  ${}^4\text{He}$  and  ${}^{16}\text{O}$ , given numerically in the LIT-CC theory by the difference  $m_0^1(q) - \bar{m}_0^1(q)$ , along with their  $K_{\text{CoM}}^1(q)$  functions given by Eq. (30) and obtain an excellent agreement. For the employed interaction  $\text{N}^3\text{LO-EM}$ , it was shown in Ref. [21] that the frequency  $\hbar\tilde{\omega}$  of  $|0_{\text{CoM}}\rangle$  is close to 19 MeV for  ${}^4\text{He}$  and 16 MeV for  ${}^{16}\text{O}$ , respectively, in the  $\Lambda\text{-CCSD(T)}$  approximation. We therefore varied the frequencies  $\hbar\tilde{\omega}$  in a range of  $\pm 1$  MeV around these values. The agreement shown in Fig. 4 can only be obtained for this narrow range for which the ground state approximately factorizes into intrinsic and CoM wave functions, further supporting our ansatz for the form of  $|f_{\text{CoM}}^J\rangle$ . We would like to emphasize here that the frequency  $\hbar\tilde{\omega} = 20$  MeV for  ${}^4\text{He}$  coincides with the value employed to obtain  $F_{\text{el}}(q)$ ; see Fig. 1. Similarly, the best agreement is obtained with  $\hbar\tilde{\omega} = 16$  MeV for  ${}^{16}\text{O}$ .

Although the analysis in this section was performed only the with  $\text{N}^3\text{LO-EM}$   $NN$  interaction, we have verified that when using  $\text{NNLO}_{\text{sat}}$ , which includes  $3N$  forces, the arguments presented here are still valid.

<sup>1</sup>This would be exactly equal to  $Z^2 |F_{\text{el}}(q)|^2$  if radial excitations were included [39].

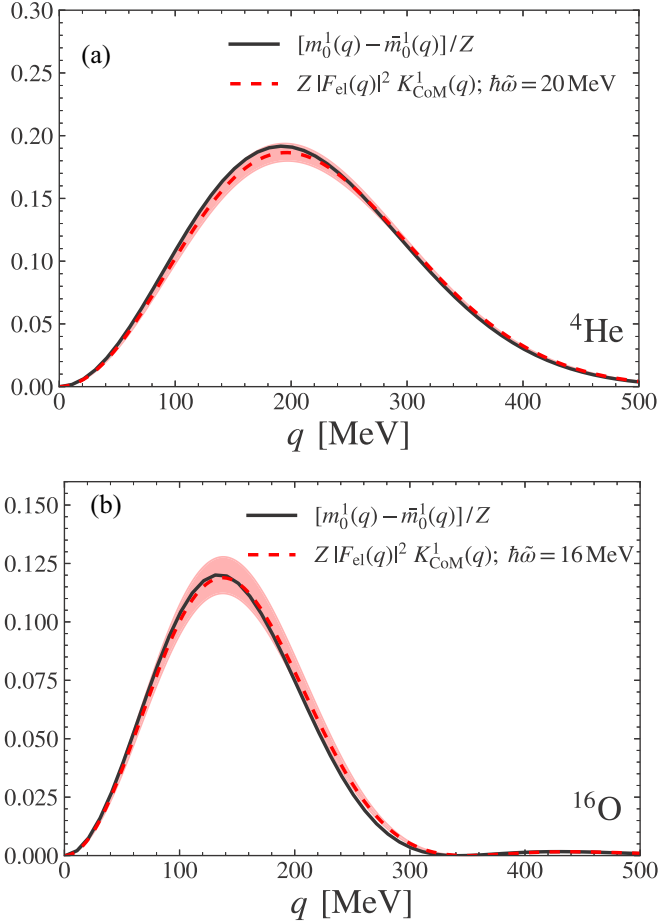


FIG. 4. Spurious states  $1^-$  for  ${}^4\text{He}$  (a) and  ${}^{16}\text{O}$  (b) compared with an ansatz for the CoM function from Eq. (30). The band for  ${}^4\text{He}$  is obtained with  $\hbar\tilde{\omega} = 20 \pm 1$  MeV. For  ${}^{16}\text{O}$  the band corresponds to  $\hbar\tilde{\omega} = 16 \pm 1$  MeV.

## VI. COMPARISON WITH OTHER CALCULATIONS AND EXPERIMENT

Finally, we compare the total CSR calculated from coupled-cluster theory with other available calculations and experimental data. At this stage we include a small effect coming from the nucleon form-factor by rewriting Eq. (4):

$$\rho(q) = \sum_{j=1}^A G_E^p(Q^2) \frac{1 + \tau_3}{2} e^{iqz_j} + G_E^n(Q^2) \frac{1 - \tau_3}{2} e^{iqz_j}, \quad (33)$$

where  $(1 \pm \tau_3)/2$  are the projectors acting in the isospin space, and  $Q^2 \approx q^2 - \omega_{QE}^2$  with the energy transfer  $\omega_{QE} = q^2/2m$  corresponding to the quasielastic peak, where  $m$  is the mass of the nucleon. We use Kelly's parametrization of  $G_E^{n,p}$  form factors [43], and also account for the Darwin-Foldy relativistic correction by including a factor of  $1/[1 + Q^2/(4m^2)]$ , while neglecting the smaller spin-orbit contribution.

In Fig. 5, we present the CSR of  ${}^4\text{He}$  and  ${}^{16}\text{O}$  for the  $\text{N}^3\text{LO-EM}$  and  $\text{NNLO}_{\text{sat}}$  interactions, respectively. The  $\text{NNLO}_{\text{sat}}$  interaction accurately reproduces the binding energy and charge radius of  ${}^{16}\text{O}$ , and we therefore focus on this interaction when comparing with experiment and with other

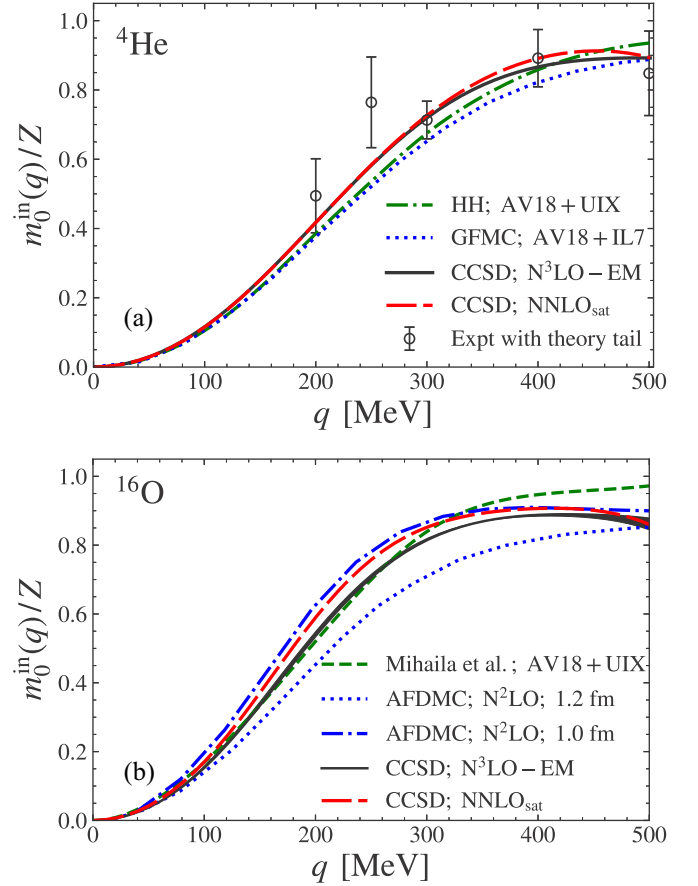


FIG. 5. (a) CSR for  ${}^4\text{He}$  in comparison to other calculations of Ref. [15] (AV18+UIX potential) and Ref. [20] (AV18+IL7 potential) together with experimental data from Refs. [40,41]. (b) CSR for  ${}^{16}\text{O}$  in comparison to other calculations by Mihaila *et al.* [18] (AV18+UIX potential) and by Lonardon *et al.* [42] (with local chiral interactions; see text for details).

theoretical approaches that use chiral  $NN$  and  $3N$  forces. We noticed a slower convergence with respect to the number of oscillator shells in the  $\text{NNLO}_{\text{sat}}$  calculations than in the  $\text{N}^3\text{LO-EM}$  calculations at large values of momentum transfer. The  $\text{NNLO}_{\text{sat}}$  results shown in Fig. 5 are for  $\hbar\tilde{\omega} = 16$  MeV and 15 major oscillator shells. By extrapolating the observed convergence pattern at smaller model spaces, we expect the calculations to be converged at  $q < 400$  MeV. At larger values of  $q$ , the basis truncation error in CSR for the  $\text{NNLO}_{\text{sat}}$  interaction is expected to be up to a few percent.

For  ${}^4\text{He}$  we compare our CCSD calculations against the HH results of Ref. [15] obtained with the AV18+UIX potential and the Green's function Monte Carlo (GFMC) results of Refs. [20] obtained with the AV18+IL7 potential. Although Ref. [20] also included the two-body charge operator, it contributes noticeably to the CSR of  ${}^4\text{He}$  only beyond the range of momenta considered in this study [44]. We see that overall the curves provide a consistent trend and we note that the dependence on the implemented Hamiltonian can be interpreted as an overall theoretical uncertainty.

Regarding  ${}^4\text{He}$ , measurements for the longitudinal response functions at intermediate momentum transfer have been performed in the past and are collected in Ref. [40], while low momentum data at  $q = 200$  and  $250$  MeV/ $c$  are taken from Buki *et al.* [41]. Since finite maximal values of the energy transfer  $\omega_{\text{max}}$  are measured in experimental data, the experimental CSR is obtained as [45]

$$m_0^{\text{in}}(q) = \frac{1}{Z} \int_{\omega_{\text{th}}^+}^{\omega_{\text{max}}} d\omega \frac{R_L(\omega, q)}{G_E^{p^2}(Q^2)} + m_{0, \text{tail}}^{\text{in}}, \quad (34)$$

where  $m_{0, \text{tail}}^{\text{in}}$  is taken from the theoretical calculations of  ${}^4\text{He}$  response functions of Ref. [13]. We notice that the experimental trend is well reproduced by all calculations of the CSR.

Our results for the CSR of  ${}^{16}\text{O}$  are compared with other theoretical calculations in panel (b) of Fig. 5. The auxiliary field diffusion Monte Carlo (AFDMC) calculations [42,44] used local chiral interactions up to next-to-next-to-leading order ( $\text{N}^2\text{LO}$ ) which were regularized in coordinate space with two different cutoff values,  $R_0 = 1.0$  and  $1.2$  fm. The coupled-cluster calculation of Mihaila and Heisenberg [18] does not include the Darwin-Foldy correction, which would reduce their CSR by as much as 5% in the  $q \approx 500$  MeV region and bring it closer to ours. Further analyses that account for uncertainties due to the interactions and the many-body methods employed are necessary to assess whether the CSR obtained using different theoretical approaches are consistent with each other within those uncertainties. Precise experimental data, especially in case of  ${}^{16}\text{O}$  for which no data exist, can constrain Hamiltonians and many-body methods used in theoretical calculations, and would therefore be very useful.

## VII. CONCLUSIONS

In this paper, we compute the CSR from coupled-cluster theory for  ${}^4\text{He}$  and  ${}^{16}\text{O}$  using  $\chi\text{EFT}$  interactions. For the first time, we investigate higher momentum transfers regime with these potentials. Through a benchmark with few-body methods, we show that the coupled-cluster wave functions retain the relevant correlations across a broad range of momentum transfer, even in the CCSD scheme. This is a very promising result because accurate treatment of nuclear correlations in the nuclear electroweak currents in this range of momentum transfers is important for improving our understanding of neutrino scattering.

Furthermore, we devise a practical method to remove the spurious states when working in the laboratory frame, and we show that the method works within a precision of a few percent. This is encouraging when moving to heavier nuclei of interest to neutrino experiments like  ${}^{40}\text{Ar}$ , where center-of-mass effects are expected to be smaller. We provide an analysis of the dominant spuriousities we remove, and find that these are excited states of a harmonic oscillator with zero radial excitation and angular excitation equal to  $J = 1$ .

Finally, we compare our results obtained with the  $\text{N}^3\text{LO-EM}$  and  $\text{NNLO}_{\text{sat}}$  potentials with other theoretical results available in the literature. In the case of  ${}^4\text{He}$ , we compare also to experimental data, which we obtained from integrating the longitudinal response function published in Refs. [40,41], and found a nice agreement. In the case of  ${}^{16}\text{O}$  no data exist for the CSR, and we find some sensitivity to the employed Hamiltonian.

This computation of the CSR in coupled-cluster theory constitutes, indeed, a first important step towards applying this method to neutrino physics in a broader research program.

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