

## First Principles Description of the Giant Dipole Resonance in $^{16}\text{O}$

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We present a calculation of the giant dipole resonance in  $^{16}\text{O}$  based on a nucleon-nucleon ( $NN$ ) interaction from chiral effective field theory that reproduces  $NN$  scattering data with high accuracy. By merging the Lorentz integral transform and the coupled-cluster methods, we extend the previous theoretical limits for breakup observables in light nuclei with mass numbers ( $A \leq 7$ ) and address the collective giant dipole resonance of  $^{16}\text{O}$ . We successfully benchmark the new approach against virtually exact results from the hyperspherical harmonics method in  $^4\text{He}$ . Our results for  $^{16}\text{O}$  reproduce the position and the total strength (bremsstrahlung sum rule) of the dipole response very well. When compared to the cross section from photoabsorption experiments, the theoretical curve exhibits a smeared form of the peak. The tail region between 40 and 100 MeV is reproduced within uncertainties.

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**Introduction.**—Giant resonances dominate the dipole response in a variety of self-bound quantum systems such as nuclei [1], atomic clusters [2], and fullerenes [3]. In photo-nuclear cross sections, the giant resonance is a very pronounced peak at about 10–20 MeV. After its first observation in uranium by Baldwin and Klaiber in 1947 [4], this prominent structure has been observed across the nuclear table. The first theoretical interpretations were given by Goldhaber and Teller [5], who proposed that the peak had to be of dipole nature [hence the name giant dipole resonance (GDR)], and by Steinwedel and Jensen [6]. The resonance was ascribed to the collective motion of protons against neutrons, and its width to the transfer of energy from this vibration into other modes of the nuclear motion [7,8]. Since then, the GDR has been the object of numerous theoretical studies trying to account for the GDR centroid and width in collective as well as microscopic many-body approaches. Self-consistent mean field theories have been extensively applied to the description of GDR (see, e.g., Refs. [9,10] for recent reviews). The effects of the continuum (pioneered in Ref. [11]) and of the particle-phonon coupling (see, e.g., Refs. [12,13]) have been studied. However, in these calculations, the dynamics is described by effective interactions which are fitted to medium-mass nuclei.

First principles continuum computations of the GDR, where one starts from interactions that reproduce nucleon-nucleon ( $NN$ ) phase shifts, are only available for nuclei with mass numbers  $A \leq 7$ . The reason is that one not only needs to account for complicated ground-state correlations, but in principle the many-body scattering problem must also be solved. In few-body calculations, these challenges were overcome by employing the Lorentz integral transform (LIT) [14,15]. This method reduces the continuum problem to a

bound-state-like problem and thereby overcomes one of the main challenges. The few-body bound-state problem was solved with the hyperspherical harmonics (HH) expansion [16,17] and the no-core shell model [18]. Starting from semi-realistic  $NN$  interactions, this approach computed the “resonant shape” of the photonuclear cross section of  $^4\text{He}$  [19,20],  $^6\text{Li}/^6\text{He}$  [21,22], and  $^7\text{Li}$  [23]. For  $^4\text{He}$ , modern realistic two- and three-body forces were also employed [24,25].

The studies of the  $A = 6$  isotopes [21,22] showed that the halo structure of the rare isotope  $^6\text{He}$  differs considerably from the stable  $^6\text{Li}$  nucleus. In  $^6\text{He}$ , the dipole cross section exhibits two well separated peaks, while a single resonant shape is observed for  $^6\text{Li}$ . These results do not depend on the employed  $NN$  interaction. It is interesting to extend such studies to heavier exotic nuclei such as the neutron-rich isotopes of oxygen and calcium. The dipole cross sections of exotic oxygen isotopes show fragmented low-lying strengths and thereby differ from the stable  $^{16}\text{O}$  [26,27]. The first step towards this goal is the extension of the *ab initio* LIT method to heavier systems. In this Letter, we combine the LIT with the coupled-cluster (CC) method [28,29] and microscopically compute the GDR for  $^{16}\text{O}$ . Our calculation employs  $NN$  interactions from chiral effective field theory [30,31], where no parameter is fit to nuclear data with  $A > 2$ .

**Method.**—The inclusive response function, also called the dynamical structure function, to a dipole excitation is defined as

$$S(\omega) = \frac{1}{2J_0 + 1} \sum_f |\langle \psi_0 | \hat{D}_0 | \psi_f \rangle|^2 \delta(E_f - E_0 - \omega). \quad (1)$$

Here,  $\omega$  is the excitation energy,  $J_0$  is the nuclear ground-state spin, while  $\psi_0$  and  $\psi_f$  denote the ground- and final-state

wave functions with energies  $E_0$  and  $E_f$ , respectively. The translationally invariant dipole operator is

$$\hat{\mathbf{D}} = \sum_i^A P_i(\mathbf{r}_i - \mathbf{R}_{\text{cm}}) = \sum_i^A \left( P_i - \frac{Z}{A} \right) \mathbf{r}_i. \quad (2)$$

Here,  $\mathbf{r}_i$  and  $\mathbf{R}_{\text{cm}}$  are the coordinates of the  $i$ th particle and the center of mass, respectively, while  $P_i$  is the proton projection operator and  $Z$  is the number of protons. In Eq. (1),  $\hat{D}_0$  indicates the component of  $\hat{\mathbf{D}}$  along the direction of the photon propagation and  $\sum_f$  stands for both a sum over discrete energy levels and an integration over continuum eigenstates. For  $A > 3$ , one faces the problem that when  $\psi_f$  is in the continuum, it cannot be calculated in an exact way at every excitation energy. Thus, a direct calculation of  $S(\omega)$  is not possible, unless one introduces approximations. However, via the LIT method, the problem can be reformulated in such a way that the knowledge of  $\psi_f$  is not necessary. To this end, one introduces the LIT of the response function as

$$L(\omega_0, \Gamma) = \int_{\omega_{\text{th}}}^{\infty} d\omega \frac{S(\omega)}{(\omega - \omega_0)^2 + \Gamma^2}. \quad (3)$$

Here,  $\omega_{\text{th}}$  is the threshold energy and  $\Gamma > 0$  is the Lorentzian width, which plays the role of a resolution parameter. By using the closure relation, one finds

$$L(z) = \langle \psi_0 | \hat{D}_0^\dagger \frac{1}{\hat{H} - z^*} \frac{1}{\hat{H} - z} \hat{D}_0 | \psi_0 \rangle = \langle \tilde{\psi} | \tilde{\psi} \rangle, \quad (4)$$

where we introduced the complex energy  $z = E_0 + \omega_0 + i\Gamma$ . The LIT of the response function  $L(z)$  can be computed directly by solving the Schrödinger-like equation

$$(\hat{H} - z) | \tilde{\psi} \rangle = \hat{D}_0 | \psi_0 \rangle \quad (5)$$

for different values of  $z$ . The solution  $| \tilde{\psi} \rangle$  has bound-state-like asymptotics; thus,  $L(z)$  can be calculated even for  $A > 3$  with any good bound-state technique. Results for  $S(\omega)$  are typically obtained from a numerical inversion [32–34] of the LIT (3) and should be independent on the choice of  $\Gamma$ .

We are interested in computing the dipole response for  $^{16}\text{O}$ . To this end, we merge the LIT with the CC method [28,29,35], which is a very efficient bound-state technique, applied with success on several medium-mass nuclei [36–40]. In CC theory, the ground state of the system is given by  $| \psi_0 \rangle = \exp(T) | \phi_0 \rangle$ . Here,  $| \phi_0 \rangle$  is a Slater determinant and  $T$  generates particle-hole ( $ph$ ) excitations. One has  $T = T_1 + T_2 + \dots$ , as the sum of a  $1p$ - $1h$  operator  $T_1$ , a  $2p$ - $2h$  operator  $T_2$ , etc. In what follows, we will consider only an expansion up to  $T_2$ , which is known as coupled clusters with singles and doubles (CCSD) [29]. In CC theory, the LIT of the dipole response function is

$$L(z) = \langle 0_L | \bar{D}_0^\dagger \frac{1}{\bar{H} - z^*} \frac{1}{\bar{H} - z} \bar{D}_0 | 0_R \rangle = \langle \tilde{\psi}_L | \tilde{\psi}_R \rangle. \quad (6)$$

Here,  $\bar{H} = \exp(-T) \hat{H} \exp(T)$  is the similarity-transformed Hamiltonian, and  $\bar{D}_0^{(\dagger)} = \exp(-T) \hat{D}_0^{(\dagger)} \exp(T)$  is the

similarity-transformed dipole (dagger) operator. The states  $\langle 0_L |$  and  $| 0_R \rangle$  are the left and right ground states of the non-Hermitian Hamiltonian  $\bar{H}$ , respectively. In analogy to Eq. (5), we compute the LIT of the response function by solving a right Schrödinger-like equation

$$(\bar{H} - z) | \tilde{\psi}_R(z) \rangle = \bar{D}_0 | 0_R \rangle \quad (7)$$

and an equivalent left Schrödinger-like equation for  $\langle \tilde{\psi}_L(z) |$ . Here,  $| \tilde{\psi}_R(z) \rangle = R(z) | \phi_0 \rangle$ , and the operator  $R$  is a linear expansion in particle-hole excitations

$$R(z) = R_0 + \sum_{ia} R_i^a \hat{c}_a^\dagger \hat{c}_i + \frac{1}{4} \sum_{ijab} R_{ij}^{ab} \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_j \hat{c}_i + \dots \quad (8)$$

To be consistent with the CCSD approximation, we truncate  $R(z)$  at the  $2p$ - $2h$  excitation level. It is implied that sums over  $i, j$  ( $a, b$ ) run over occupied (unoccupied) states. An equivalent expansion can be written for the left excitation operator. The LIT of Eq. (6) can be computed efficiently by employing a generalization of the Lanczos algorithm for nonsymmetric matrices. In our calculations, we use a  $NN$  interaction from chiral effective field theory at next-to-next-to-next-to-leading order [41], supplemented by a point Coulomb force. We omit three-nucleon (3N) forces that already appear at next-to-next-to-leading order [42] due to the problems associated with computing 3N forces in the large model spaces we employ. Note that 3N forces have a smaller impact on the photoabsorption cross section of  $^4\text{He}$  [24] (few percent in the peak), but it is not clear how large their effect is for  $^{16}\text{O}$ .

*Benchmark for  $^4\text{He}$ .*—For quality assurance, we want to compare the CC results with virtually exact results obtained from the effective interaction hyperspherical harmonics (EIHH) method [16] for  $^4\text{He}$ . Figure 1(a) shows  $L(\omega_0, \Gamma)$  at fixed  $\Gamma = 10$  MeV, computed with the CC method in model spaces with  $\hbar\Omega = 20$  MeV and  $N_{\text{max}} = 2n + l = 8, 10, 12, \dots, 18$ . The results are well converged in large model spaces with  $N_{\text{max}} = 18$ . Figure 1(b) shows a comparison with EIHH results. The CCSD calculation is based on a model space with  $N_{\text{max}} = 18$  and  $\hbar\Omega = 20$  MeV and agrees very well with the EIHH result. In these large model spaces, the CCSD results are practically independent of the oscillator frequency. We attribute the small differences to the truncation inherent in the CCSD approximation.

It is also interesting to compare the two  $S(\omega)$  obtained, inverting the CCSD and HH results for the LIT. For the inversion, we use the minimization procedure of Refs. [32,33] and require the solutions of this ill-posed problem to be zero below the threshold energy  $\omega_{\text{th}}$ . The latter is the difference between the binding energies of  $^4\text{He}$  and  $^3\text{He}$ , being  $\gamma + ^4\text{He} \rightarrow ^3\text{He} + p$  the first open reaction channel in the inclusive process. For the next-to-next-to-next-to-leading-order two-body potential, the binding energies are 23.97 (7.37) MeV obtained within the CCSD approximation and the particle-removed equation-of-motion method [37,43], and 25.39 (7.85) MeV with EIHH

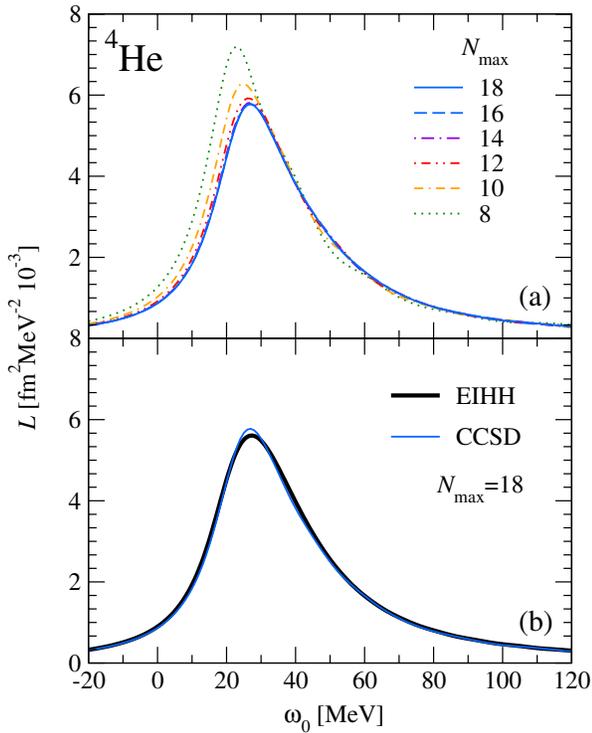


FIG. 1 (color online). LIT for  $\Gamma = 10$  MeV. (a) Convergence with  $N_{\max}$  of the CCSD result with  $\hbar\Omega = 20$  MeV. (b) Comparison between CCSD and HH results.

for  $^4\text{He}$  ( $^3\text{He}$ ), respectively. Figure 2 shows the comparison of the response functions from the CC and EIHH methods. The exact threshold energy  $\omega_{\text{th}} = 17.54$  MeV has been used in all the inversions. For the CCSD calculations, we used a model space with  $N_{\max} = 18$  and  $\hbar\Omega = 20$  MeV. We found that the inversions are insensitive to  $\hbar\Omega$ . The band for the CCSD curve results from inverting the LIT with  $\Gamma = 10$  MeV and  $\Gamma = 20$  MeV and estimates the numerical uncertainty associated with the inversion. For the EIHH results, the inversions of the LIT with  $\Gamma = 10$  and

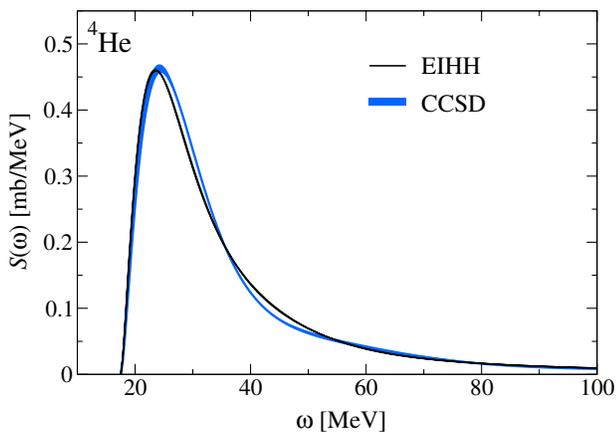


FIG. 2 (color online). Comparison of the  $^4\text{He}$  dipole response function calculated with CCSD ( $\hbar\Omega = 20$  MeV and  $N_{\max} = 18$ ) with the EIHH result.

20 MeV overlap. The CCSD response function is close to the virtually exact EIHH result. Apparently, the small deviations between the CCSD and the exact result for the LIT in Fig. 1(b) translate into small deviations in the response function for energies between about  $\omega = 30$  and 50 MeV.

The  $^4\text{He}$  benchmark suggests that the CC method can be employed for the computation of the dipole response and that theoretical uncertainties are well controlled. This makes it exciting to apply the CC method for the computation of the giant dipole resonance of  $^{16}\text{O}$ .

*Extension to  $^{16}\text{O}$ .*—Figure 3(a) shows the convergence of the CCSD LIT for  $\Gamma = 10$  MeV and a sequence of model spaces with  $\hbar\Omega = 26$  MeV and  $N_{\max}$  from 8 up to 18. The convergence is good, and small differences between  $N_{\max} = 16$  and  $N_{\max} = 18$  are only visible close to the maximum. We recall that the convergence of the LIT also depends on the choice of the resolution parameter  $\Gamma$ . A faster convergence is achieved for increasing  $\Gamma$ . In what follows, we show  $\Gamma = 10$  MeV, the smallest width giving a good convergence.

It is interesting to compare our result of the LIT with data. The experiment by Ahrens *et al.* [44] measured the total photoabsorption cross section  $\sigma_\gamma$  on an oxygen target with natural abundance (99.762%  $^{16}\text{O}$ ) with an attenuation method. In the unretarded dipole approximation, the cross section is related to  $S(\omega)$  of Eq. (1) via ( $\alpha$  is the fine structure constant)

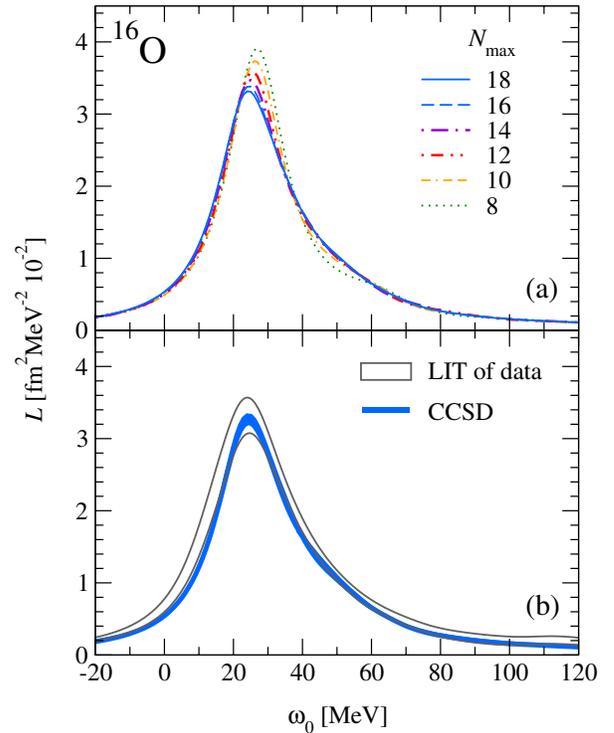


FIG. 3 (color online). (a) Convergence of  $L(\omega_0, \Gamma)$  at  $\Gamma = 10$  MeV as a function of  $N_{\max}$  for  $\hbar\Omega = 26$  MeV. (b) Comparison of the LIT at  $\Gamma = 10$  MeV within CCSD for  $N_{\max} = 18$  and the Lorentz integral transform of Ahrens *et al.* data [44].

$$\sigma_\gamma(\omega) = 4\pi^2 \alpha \omega S(\omega). \quad (9)$$

We extract  $S(\omega)$  from the cross-section data and apply the LIT of Eq. (3) to the experimental  $S(\omega)$ . This allows a direct comparison with theory, avoiding the inversion procedure. Figure 3(b) shows such a comparison. The band spanned by the experimental data results from Lorentz transforming the data with the corresponding error bars. The band of the CCSD results is obtained by varying the harmonic oscillator (HO) frequency between  $\hbar\Omega = 20$  and 26 MeV. The theoretical and experimental results agree within the uncertainties in almost all the  $\omega_0$  range. Recall that the (normalized) Lorentzian kernel is a representation of the  $\delta$  function. Therefore, the integral in  $\omega_0$  of  $L(\omega_0, \Gamma)$  is the same as the integral in  $\omega$  of  $S(\omega)$ . Also, peak positions are approximately conserved. Thus, from the agreement of the LITs, we can already anticipate that the theoretical results well reproduce the experimental centroid and total strength (bremsstrahlung sum rule).

Finally, we perform the inversion of the computed LIT and confront theoretical and experimental  $S(\omega)$ . For the inversion, we make the following ansatz:

$$S(\omega) = \omega^{3/2} \exp\left(-\alpha Z_1 Z_2 \sqrt{\frac{2\mu}{\omega}}\right) \sum_i^N c_i e^{-\omega/\beta_i}. \quad (10)$$

Here, the exponential prefactor is a Gamow factor, and  $\mu \sim (A - 1/A)m_n$  is the reduced mass, with  $m_n$  being the nucleon mass. The charges  $Z_1 = 7$  and  $Z_2 = 1$  correspond to the first disintegration channel (proton separation) in the  $\gamma + {}^{16}\text{O}$  reaction. The binding energy and  $\omega_{\text{th}}$  in the CCSD approximation (experiment) are 107.24 (127.72) and 14.25 (12.13) MeV, respectively. The threshold energy  $\omega_{\text{th}}$  is computed within coupled-cluster theory using the particle-removed equation of motion [29]. Note that the inversion is sensitive to numerical noise and that the CCSD results using the HO basis are (only) converged at a few-percent level and not at an ideal subpercent level. In order to improve the convergence and make the inversion more stable, we employ a basis of bound and discretized continuum states obtained from diagonalizing a spherical Woods-Saxon potential in a discrete plane-wave basis of 35 mesh points for the proton and neutron  $d_{5/2}$ ,  $s_{1/2}$ ,  $d_{3/2}$  partial waves [45]. For the remaining partial waves, we employed  $N_{\text{max}} = 16$  HO shells with  $\hbar\Omega = 26$  MeV. The inversion determines the coefficients  $c_i$  and the nonlinear parameter  $\beta$  of the  $N$  basis functions by a least-square fit. Figure 4 shows the CCSD dipole response function and compares it to the data of Ahrens *et al.* [44] and also to the more recent evaluation by Ishkhanov *et al.* [46,47]. The theoretical band is obtained by inverting the LIT with width  $\Gamma = 10$  MeV and by varying the number  $N$  of basis functions employed in the inversion from 5 to 9. By inverting the LIT at  $\Gamma = 20$  MeV, we get very similar results. The band is a lower estimate of the theoretical error, as it does not account, e.g., for missing triples in the cluster

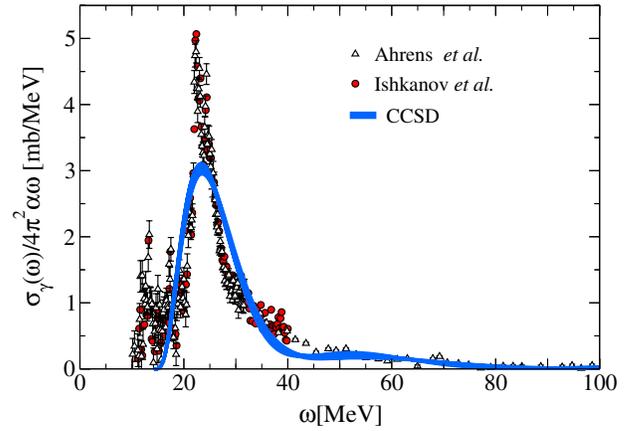


FIG. 4 (color online). Comparison of the  ${}^{16}\text{O}$  dipole response calculated in the CCSD scheme against experimental data by Ahrens *et al.* [44] (triangles with error bars) and Ishkhanov *et al.* [46] (red circles).

expansion. The position of the GDR in  ${}^{16}\text{O}$  is nicely explained by our calculation, whose only ingredient is a  $NN$  interaction which fits  $NN$  scattering data. That is the case, despite the fact that the binding and threshold energies are not correctly reproduced. This fact might be coincidental, given that we are omitting 3N forces, which may have an impact on the response function. We observe that the form of the theoretical result is somewhat smeared, compared to data. If larger model spaces were available to allow a more accurate calculation of the LIT at  $\Gamma = 10$  and even at smaller  $\Gamma$ , then finer structures in the response could be possibly resolved, if present. The more structured form of the data below 20 MeV can be due to the contribution of higher multipoles (quadrupole and octupole) in the photoabsorption cross section. We note that the tail region between 40 and 100 MeV is reproduced within uncertainties. When integrating the theoretical photoabsorption cross section up to 100 MeV, we obtain an enhancement  $\kappa = 0.57\text{--}0.58$  of the Thomas-Reiche-Kuhn sum rule [59.74( $NZ/A$ ) MeV mb(1 +  $\kappa$ )].

*Summary.*—We develop a new method based on merging the Lorentz integral transform approach with coupled-cluster theory, which opens up important perspectives for studying physical phenomena involving the continuum, also in other fields. For example, with the present approach, one could explore problems in quantum chemistry, where the CC method is largely used but the continuum is often discretized. As a first application in nuclear physics, we present a calculation of the GDR in  ${}^{16}\text{O}$ , starting from a  $NN$  interaction from chiral effective field theory that reproduces  $NN$  scattering data with high accuracy. We compute the Lorentz integral transform of the dipole response function with the CCSD scheme. An inversion of the transform yields the dipole response function. The theoretical result reproduces the experimental centroid as well as the total dipole strength (bremsstrahlung sum rule) very well and exhibits a somewhat smeared shape compared to the data. This work is a first

important step towards an *ab initio* description of the electromagnetic responses of medium-heavy stable and rare isotopes from full chiral Hamiltonians.

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