Ab initio calculations of electric dipole moments of light nuclei

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(Dated: August 23, 2021)

In any finite system, the presence of a non-zero permanent electric dipole moment (EDM) would indicate CP violation beyond the small violation predicted in the Standard Model. Here, we use the ab initio no-core shell model (NCSM) framework to theoretically investigate the magnitude of the EDM of the nucleus. We calculate EDMs of several light nuclei using chiral two- and three-body interactions and a PT-violating Hamiltonian based on a one-meson-exchange model. We present a benchmark calculation for \(^{3}\)He, as well as results for the more complex nuclei \(^{6,7}\)Li, \(^{9}\)Be, \(^{10,11}\)B, \(^{13}\)C, \(^{14,15}\)N, and \(^{19}\)F. Our results suggest that different nuclei can be used to probe different terms of the PT violating interaction. These calculations allow us to suggest which nuclei may be good candidates in the search for a measurable permanent electric dipole moment.

I. INTRODUCTION

A permanent electric dipole moment (EDM) of a physical system would indicate direct violation of time-reversal (T) and parity (P) and thus charge conjugation and parity (CP) violation through the CPT invariance. CP violation is a required condition for baryogenesis in the early universe [1]. In the Standard Model (SM) with three generations of quarks, CP is broken by the phase of the Cabibbo-Kobayashi-Maskawa (CKM) mixing matrix [2] and by the QCD \(\theta\) term [3]. While observed CP violation in the kaon and B meson systems can be explained by the CKM mechanism, CP violation in the SM fails to generate the observed matter-antimatter asymmetry of the Universe by several orders of magnitude [4, 5].

The CKM mechanism predicts values for the EDMs of leptons, nucleons, atomic and molecular systems that are too small to be detected in the foreseeable future, and hence a measured nonzero EDM in any of these systems is an unambiguous signal for a new source of CP violation and for physics beyond the SM [6]. The present experimental upper bounds on the EDMs of neutron and proton are \(|d_n|<1.8 \times 10^{-13}\) e fm [7] and \(|d_p|<2 \times 10^{-12}\) e fm, where the proton EDM has been inferred from a measurement of the diamagnetic \(^{199}\)Hg atom [8]. For the electron, the most recent upper bound is \(|d_e|<8.7 \times 10^{-16}\) e fm [9], derived from the EDM of the ThO molecule.

In this letter, we focus on nuclear EDMs. There are proposals to measure the EDMs of charged particles, including protons and light nuclei, in dedicated storage ring experiments [10–13]. These experiments might reach a sensitivity of \(10^{-16}\) e fm, comparable with the next generation of neutron EDM experiments. Unlike searches for CP-violating moments of the nucleus through measurements of atomic EDMs, a measurement for a stripped nucleus would not suffer from a suppression of the signal through atomic Schiff screening [14]. In comparison to a proton or a neutron EDM, EDMs of atomic nuclei can be enhanced by many-body effects [15].

EDMs of few nucleon systems, the deuteron, \(^3\)H, \(^3\)He, have been investigated by various ab initio approaches [16–23] using phenomenological meson-exchange and/or chiral Effective Field Theory (EFT) interactions as well as within pionless EFT framework [24]. Recently, EDMs of selected \(p\)-shell nuclei were calculated within the cluster model [25–30]. In particular, EDMs were reported for \(^6\)Li [25], \(^3\)Be [29], \(^7\)Li and \(^{11}\)B [30], and \(^{13}\)C [26] using phenomenological cluster-cluster PT-conserving (PTC) interaction and one-meson-exchange based PT-violating (PTV) nucleon-nucleon (NN) interaction.

In this work, we perform ab initio calculations of EDMs for light nuclei within the no-core shell model (NCSM) [31–33] framework using chiral NN and three-nucleon (3N) PTC interactions and one-meson-exchange PTV NN interactions as the only input. The NCSM is applicable in a universal way to few-nucleon systems, \(p\)-shell, and light \(sd\)-shell nuclei. We present benchmark calculations for \(^3\)He as well as results for the more complex stable nuclei \(^{6,7}\)Li, \(^{9}\)Be, \(^{10,11}\)B, \(^{13}\)C, \(^{14,15}\)N, and \(^{19}\)F. We note that NCSM was applied to obtain the first ab initio EDM results for \(^3\)He and \(^9\)H in Refs. [17] and [19], respectively.

II. NO-CORE SHELL MODEL

In the NCSM, nuclei are described as systems of \(A\) non-relativistic point-like nucleons interacting through realistic inter-nucleon interactions. All nucleons are active degrees of freedom. The many-body wave function is cast into an expansion over a complete set of antisymmetric \(A\)-nucleon harmonic oscillator (HO) basis states containing up to \(N_{\text{max}}\) HO excitations above the

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lowest Pauli-principle-allowed configuration. The basis is further characterized by the frequency $\Omega$ of the HO well. Square-integrable energy eigenstates are obtained by solving the Schrödinger equation

$$H |A \lambda I^\pi\rangle = E_k^I |A \lambda I^\pi\rangle$$

with the intrinsic PTC Hamiltonian

$$H = \frac{1}{A} \sum_{i<j=1}^{A} (\tilde{p}_i^2 - \tilde{p}_j^2)/2m + \sum_{i<j=1}^{A} V_{ij}^{NN} + \sum_{i<j<k=1}^{A} V_{ijk}^{3N},$$

Here, $m$ is the nucleon mass, $\tilde{p}$ nucleon momenta, $V^{NN}$ and $V^{3N}$ PTC NN and 3N interaction, respectively. The $\lambda$ in (1) labels eigenstates with identical $I^\pi$. The eigenstates of $H$ (2) can be also characterized by isospin quantum number $T$ that is typically conserved to a good approximation. We note, however, that our calculations fully include isospin breaking originating from the Coulomb interaction and strong force contributions present in the $V^{NN}$.

The present calculations are performed using the Slater determinant (SD) HO basis in the so-called $M$-scheme where the basis is characterized by $A$, the projection $I_0$ of the total angular moment $I$, parity $\pi$ and $T_z=(Z-N)/2$ with $Z$ and $N$ the proton and neutron number, respectively. Only the eigenstates (1) obtained by diagonalization using the Lanczos algorithm have good $I$ and approximately good $T$. They factorize exactly as products of physical intrinsic eigenstates and a center-of-mass state in the $0\hbar \Omega$ excitation.

In the present work we adopt the NN+3N chiral interaction applied in Ref. [34], denoted as NN+3N(inl), consisting of an NN interaction up to the fourth order ($N^3LO$) in the chiral expansion [35] and a 3N interaction up to next-to-next-to-leading order ($N^2LO$) using a combination of local and non-local regulators. Even though all the underlying parameters (known as low-energy constants or LECs) are determined in $A=2,3,4$ nucleon systems, this interaction provides a very good description of properties of both light and medium mass nuclei [34], including $^{100}$Sn [36]. The chiral orders of the adopted NN and 3N interactions are not consistent: the former is included up to order $N^3LO$ while the latter is at $N^2LO$. While the $N^3LO$ 3N contribution has been shown to be rather small [37], the consistency of the regulator and/or in particular the use of a non-local versus local regulators plays a significant role in medium mass nuclei [38].

A faster convergence of our calculations with respect to the many-body basis size is obtained by softening the chiral interaction through the similarity renormalization group (SRG) technique [39–43]. The SRG unitary transformation induces many-body forces, included here up to the three-body level. The four- and higher-body induced terms are small at the $A_{SRG}=2.0$ fm$^{-1}$ resolution scale used in present calculations [34].

### III. THE NUCLEAR ELECTRIC DIPOLE MOMENT

A nuclear EDM consists of contributions from the intrinsic EDMs of the proton and neutron, $d_p$ and $d_n$, and from the polarization effect caused by the PTV nuclear interaction, as well as from the two-body PTV meson-exchange charge operator. The latter was found to be just a few percent of the polarization contribution for the deuteron case [16] and will not be considered in this work.

Contributions due to intrinsic EDMs of the nucleons can be evaluated by calculating the matrix element

$$D^{(1)} = \langle A \text{gs} I^\pi I_z=I | D^{(1)} | A \text{gs} I^\pi I_z=I \rangle$$

where the ground state wave function is obtained by solving the Schrödinger equation (1) with the PTC Hamiltonian (2). The $\tau$ and $\sigma$ are nucleon isospin and spin operators, respectively.

The PTV NN interaction admixes unnatural parity states in the ground state

$$|A \text{gs} I^\pi\rangle = |A \text{gs} I^\pi\rangle + \sum_\lambda \left| A \lambda I^{-\pi} \right\rangle$$

$$\times \frac{1}{E_{\text{gs}}^I - E_{\lambda}^I} \langle A \lambda I^{-\pi} | V_{\text{PTV}}^{NN} | A \text{gs} I^\pi \rangle,$$

which then gives rise to the induced EDM moment. We use the one-meson-exchange model for the PTV NN interaction including the $\pi^\pm$, $\rho^-$, and $\omega^+$ meson exchanges in the form [16, 44, 45]

$$V_{\text{PTV}}^{NN} = \frac{1}{2m} \left\{ \sigma \cdot \nabla \left( -G_0^\pi y_\omega(r) \right) + \tau_1 \cdot \tau_2 \sigma \cdot \nabla \left( G_0^\pi y_\pi(r) - G_0^\rho y_\rho(r) \right) \right\}$$

$$+ \frac{1}{2} \tau_+^z \sigma_+ \cdot \nabla \left( G_+^\pi y_\pi(r) - G_+^\rho y_\rho(r) - G_+^\omega y_\omega(r) \right)$$

$$+ \frac{1}{2} \tau_-^z \sigma_- \cdot \nabla \left( G_-^\pi y_\pi(r) + G_-^\rho y_\rho(r) - G_-^\omega y_\omega(r) \right)$$

$$+ (3\tau_1^z \tau_2^z - \tau_1 \cdot \tau_2) \sigma \cdot \nabla \left( G_x^\pi y_\pi(r) - G_x^\rho y_\rho(r) \right),$$

where $G_\lambda^\pi = g_\lambda g_{\lambda\text{NN}}$ is a product of a PTV $\chi$-meson-nucleon coupling and its associate strong one, $y_{\lambda}(r)=e^{-m_{\lambda}r}/(4\pi r)$ is the Yukawa function with a range determined by the mass of the exchanged $\chi$-meson, $\tilde{r}=\tilde{r}_1 - \tilde{r}_2$, $\tilde{\sigma}\pm=\sigma_\pm \pm \tilde{\sigma}_2$, and $\tilde{r}_\pm=\tilde{r}_1 \pm \tilde{r}_2$.

In the NCSM, when the $|A \text{gs} I^\pi\rangle$ is calculated in $N_{\text{max}}$ space, the corresponding unnatural parity states appearing in Eq. (4) are obtained in $N_{\text{max}}+1$ space. It is not necessary to compute many excited unnatural parity states as Eq. (4) suggests. Rather, first, we solve the standard Schrödinger equation (1) using the PTC Hamiltonian (2) and obtain the $|A \text{gs} I^\pi\rangle$ wave function, and
second, we invert the generalized Schrödinger equation with an inhomogeneous term,

\[ (E_{gs}^\tau - H)|A gs I\rangle = V_{NN}^{PTV}|A gs I^\tau\rangle, \quad (6) \]

to obtain the unnatural parity admixture in the ground state. The inversion is performed by the Lanczos continued fraction method [17, 46, 47].

The polarization contribution to the nuclear EDM is then calculated as

\[ D^{(pol)} = \langle A gs I^\tau I_z=I| \sum_{i=1}^{A} (1 + \tau_i^z) z_i |A gs I_z=I\rangle + \text{h.c.} \quad (7) \]

with the electric dipole moment operator projected in the z-direction. With this form of the transition operator the leading effects of two-body electromagnetic currents are included through the Siegert theorem.

IV. RESULTS AND DISCUSSION

To compute matrix elements of the \( V_{NN}^{PTV} \) interaction (5) and solve the equation (6), we adapted codes used for calculations of anapole moments of light nuclei reported in Ref. [48]. To benchmark our codes, we calculated the EDM of \(^3\)He using PTC chiral N^3LO NN interaction [35] without any renormalization as \(^3\)He EDM results for this interaction together with the PTV interaction (5) were published in Ref. [17]. The NCSM basis convergence for the polarization contribution to \(^3\)He EDM is shown in Fig. 1 and our \( D^{(1)} \) and \( D^{(pol)} \) results are summarized in Table I. The \( D^{(pol)} \) \( N_{\text{max}} \) convergence is quite satisfactory while that of \( D^{(1)} \) is still faster. In Fig. 1, the odd \( N_{\text{max}} \) values correspond to the unnatural states in Eq. (4), i.e., the largest space for the ground-state was \( N_{\text{max}}=16 \). While our \( D^{(1)} \) results agree with those reported in Ref. [17] (Table 1, the EFT NN column in that paper), the present \( D^{(pol)} \) results are smaller by a factor of 1/2 compared to Ref. [17] (Table 2, the EFT NN columns in that paper). It should be noted that the same 1/2 discrepancy was reported in Ref. [20] for the isoscalar and isovector terms, while a discrepancy of 1/5 was found for the isotensor terms. Similarly, a factor of 1/2 difference was found in Ref. [25] although for all the terms. Our results are then consistent with those of Ref. [25]. The NCSM was applied in Ref. [17] (and also in Ref. [19]). However, the Jacobi-coordinate HO basis was employed as opposed to the SD HO basis used here, i.e., different codes were utilized. We plan to reexamine the codes used in Ref. [17] to investigate the issue further.

Basis-size convergence of the polarization contributions to the EDM for \( p \)-shell nuclei is also quite reasonable and comparable to that of the anapole moments [48]. In Fig. 2, we show the \( N_{\text{max}} \) convergence of the isovector \( \pi \)-exchange contribution for \(^6\)Li and \(^9\)Be as a representative example. Again, the odd \( N_{\text{max}} \) values correspond to the unnatural-parity states in Eq. (4). The largest

![Figure 1](image-url)  
**Figure 1.** The polarization contribution to \(^3\)He EDM (in e fm) due to the \( \pi \)-exchange PTV NN interaction (5). Dependence on the NCSM basis size characterized by \( N_{\text{max}} \) for two HO frequencies is shown. Chiral N^3LO PTC NN interaction from Ref. [35] was used.

![Figure 2](image-url)  
**Figure 2.** The polarization contribution to \(^6\)Li and \(^9\)Be EDM (in e fm) due to the isovector \( \pi \)-exchange PTV NN interaction (5). Dependence on the NCSM basis size characterized by \( N_{\text{max}} \) is shown. SRG-evolved chiral NN+3N(lnl) PTC interaction from Ref. [34] was used. The HO frequency \( \hbar \Omega=20 \) MeV was used.
Our $D^{(1)}$ and $D^{(pol)}$ results for all considered nuclei are shown in Table I. In Fig. 3, we display all the calculated polarization contributions to the EDMs of the $p$-shell stable nuclei and $^{19}$F. We can evaluate the uncertainties of our results due to the basis size convergence at about 10% to 20%. The other sources of uncertainty are renormalization and incompleteness of the transition operators and the uncertainties due to the description of the nuclear PTC and PTV forces. Although different sources of uncertainty might be at play, a rough estimate of the accuracy of our calculations can still be obtained by a comparison of the calculated and experimental magnetic moments shown in the last two columns of Table I. For $^{19}$F, we obtain in addition the magnetic moment $+3.73$ $\mu_N$ for the $5/2^+$ excited state that can be compared to the experimental $+3.607(8)$ $\mu_N$ [49]. We note that we used a one-body M1 operator. The largest discrepancies occur for $^{11}$B and $^{13}$C from which we estimate the uncertainty of our results at about 30%.

The present results for $^{6,7}\text{Li}$, $^{9}\text{Be}$, $^{11}$B, and $^{13}$C nuclei can be compared to the cluster model calculations reported in Refs. [25–30]. For $^{6}\text{Li}$, cluster model results are available for $d_p$, $d_n$, and $G^1_\rho$, whereas $\chi$ stands for $\pi$, $\rho$, or $\omega$ exchanges. In the last two columns, calculated and experimental (from Ref. [49]) nuclear magnetic dipole moments (in $\mu_N$) are compared. SRG-evolved chiral NN+$3N$(nl) PTC interaction from Ref. [34] was used except for $^3\text{He}$ where the chiral N$^4$LO PTC NN [35] was utilized.

Table I. The nucleonic and polarization contributions to EDMs of $^3\text{He}$, stable $p$-shell nuclei, and $^{13}\text{F}$ (in $\epsilon$ fm) decomposed as coefficients of $d_p$, $d_n$, and $G^0_\pi$, where $\chi$ stands for $\pi$, $\rho$, or $\omega$ exchanges. In the last two columns, calculated and experimental (from Ref. [49]) nuclear magnetic dipole moments (in $\mu_N$) are compared. SRG-evolved chiral NN+$3N$(nl) PTC interaction from Ref. [34] was used except for $^3\text{He}$ where the chiral N$^4$LO PTC NN [35] was utilized.

|          | $d_p$ | $d_n$ | $G^0_\pi$ | $G^1_\pi$ | $G^2_\pi$ | $G^0_\rho$ | $G^1_\rho$ | $G^2_\rho$ | $\mu$ | $\mu^{exp.}$ |
|----------|-------|-------|----------|----------|----------|----------|----------|----------|------|-------------|
| $^3\text{He}$ | -0.031 | 0.905 | 0.0073   | 0.011    | -0.0062  | 0.00063  | -0.0014  | 0.00042  | -0.00086 | -1.79 | -2.127      |
| $^6\text{Li}$ | 0.892 | 0.890 | 0.00006  | 0.0171   | 0.0002   | -0.000003| 0.00158  | -0.00002 | -0.00016 | +0.84 | +0.822      |
| $^7\text{Li}$ | 0.930 | 0.018 | -0.0096  | 0.0106   | -0.0233  | 0.00131  | 0.00085  | 0.0029   | -0.00072 | -0.0013 | +2.99 | +3.256      |
| $^9\text{Be}$ | 0.018 | 0.720 | 0.0007   | 0.0116   | 0.0053   | 0.00019  | 0.00005  | -0.0002  | 0.00046  | -0.0004 | -1.05 | -1.177      |
| $^{10}\text{B}$ | 0.852 | 0.848 | -0.0001  | 0.0281   | -0.0002  | 0.00001  | 0.00075  | 0.00002  | -0.00017 | +1.83 | +1.801      |
| $^{11}\text{B}$ | 0.444 | 0.050 | -0.0070  | 0.0127   | -0.0219  | 0.00039  | 0.00019  | 0.0019   | -0.00016 | -0.0010 | +2.09 | +2.689      |
| $^{12}\text{C}$ | -0.098 | -0.282 | -0.0058  | -0.0084  | -0.0316  | 0.00016  | -0.0052  | 0.0037   | 0.00004  | 0.0010 | +0.44 | +0.702      |
| $^{14}\text{N}$ | -0.366 | -0.363 | 0.0003   | -0.0172  | 0.0006   | -0.00003 | -0.00081 | -0.00001 | 0.00002  | 0.0014 | +0.37 | +0.404      |
| $^{15}\text{N}$ | -0.296 | 0.008 | 0.0102   | -0.0095  | -0.0228  | -0.0052  | -0.0044  | -0.0015  | 0.00039  | 0.0008 | -0.25 | -0.283      |
| $^{19}\text{F}$ | 0.818 | -0.052 | -0.0175  | 0.0089   | -0.0226  | 0.00236  | 0.00125  | 0.0027   | -0.00096 | -0.0014 | +2.85 | +2.629      |

V. CONCLUSIONS AND OUTLOOK

A nucleus in which a significantly enhanced $D^{(pol)}$ can be anticipated is the exotic $^{11}\text{Be}$, famous for its ground-state parity inversion and the strongest known electric dipole transition between bound states [52], with $13.8$ s half-life that can be readily produced at facilities such as ISAC/ARIEL at TRIUMF. Due to the halo nature of its ground state, the NCSM used here is not applicable as ISAC/ARIEL at TRIUMF. Due to the halo nature of its ground state, the NCSM used here is not applicable as ISAC/ARIEL at TRIUMF.
In summary, we performed \textit{ab initio} calculations of EDMs of light nuclei beyond the typically studied $A=2, 3$ systems. These calculations allow us to better understand which nuclei may have enhanced EDMs, and thus allow us to suggest which ones may be good candidates in the search for a measurable permanent electric dipole moment.

**ACKNOWLEDGMENTS**

We thank I. Stetcu for useful discussions. This work was supported by the NSERC Grant No. SAPIN-2016-00033. TRIUMF receives federal funding via a contribution agreement with the National Research Council of Canada. Computing support came from an INCITE Award on the Summit supercomputer of the Oak Ridge Leadership Computing Facility (OLCF) at ORNL, and from Westgrid and Compute Canada.

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