I. INTRODUCTION

The parity ($P$)–odd and time ($T$)–even nuclear anapole moment originates from the second-order term in the multipole expansion of the magnetic vector-potential together with the $P$– and $T$– violating magnetic quadrupole moment [1]. It provides the dominant contribution to the nuclear-spin-dependent (NSD) parity violating (PV) effect in atoms and molecules [2]. The corresponding term in the Hamiltonian arising from this NSD PV electron-nucleus interaction for a single electron is (atomic units are used throughout)

$$H_A = \kappa_{NSD} \frac{G_F}{\sqrt{2} I} \frac{\alpha \cdot I}{I} \rho(r), \quad (1)$$

where $\kappa_{NSD}$ is the dimensionless strength constant, $G_F = 2.22249 \times 10^{-14}$ a.u., the Fermi coupling constant, $\alpha$ is the vector comprised of the conventional Dirac matrices, $I$ is the nuclear spin, $r$ is the displacement of the valence electron from the nucleus, and $\rho(r)$ is the (normalized) nuclear density. The nuclear anapole moment contribution to the NSD interaction requires nuclear spin $I \neq 0$ and in a simple valence model has the following value [3]

$$\kappa_A = 1.15 \times 10^{-3} \left( \frac{\kappa}{I+1} \right) A^{2/3} \mu_m g_m. \quad (2)$$

Here, $A$ is the number of nucleons, $\kappa = (-1)^{l+\frac{1}{2}-l}(I+1/2)$, $l$ is the orbital angular momentum of the external unpaired nucleon, i.e. $m = n, p$; $\mu_p = +2.8$, $\mu_n = -1.9$. Theoretical estimates give the strength constant for nucleon-nucleus weak potential $g_p \approx +4.5$ for a proton and $g_n \approx 1$ for a neutron [4]. Since the nuclear anapole moment contribution to the NSD interaction scales with the number of nucleons, $\kappa_A \sim A^{2/3}$, it becomes the dominant contribution in spin-dependent atomic parity violation effects for sufficiently large nuclear charge $Z$ [5]. Two other contributions to the NSD interaction arise from the electroweak neutral coupling between the electron vector and the nucleon axial-vector currents ($V_v A_N$) [5] and from the nuclear-spin-independent weak interaction combined with the hyperfine interaction [6].

The nuclear anapole moment was experimentally measured in the $^{133}$Cs atom in 1997 [7], following a proposal by Flambaum and Khriplovich [2]. Further anapole measurements are however required to provide accurate values for the $g_p$ and $g_n$ constants, thus obtaining important information about hadronic weak coupling.

In Refs. [8–10] it was shown that the nuclear spin-dependent parity violation effects are enhanced by a factor of $10^5$ in diatomic molecules with $2\Sigma_{1/2}$ and $2\Pi_{1/2}$ electronic states due to the mixing of close rotational states of opposite parity ($\Omega$-doublet for $2\Pi_{1/2}$). These systems are thus advantageous for measurement of the NSD parity violation effects, and should provide data on anapole moments for many heavy nuclei. Two experimental proposals for using diatomic molecules to measure NSD parity violation effects were published in recent years [11, 12], and the corresponding experiments have already begun. An additional experiment of precision spectroscopy of the cooled SrF molecule is conducted at the University of Groningen [13]. Diatomic positive molecular ions also experience the enhancement of the NSD PV effects, and have an additional experimental advantage of being easy to trap and study at low temperatures [14]. An experiment to cool diatomic molecular ions in the $2\Sigma_{1/2}$ ground state for measurement of PV effects is currently attempted at the Northwestern University [15].

A number of theoretical investigations of the NSD parity violation in neutral diatomic molecules have been published in recent years, using both semiempirical
II. COMPUTATIONAL DETAILS

For $^2\Sigma^+_{1/2}$ and $^2\Pi_{1/2}$ electronic states considered, the interaction (1) can be replaced by the effective operator, which appears in the spin-rotational Hamiltonian [10, 11],

$$H^{\text{eff}}_A = \kappa_{\text{NSD}} W_A \left( n \times S' \right) \cdot I,$$

where $S'$ is the effective spin and $n$ is the unit vector directed along the molecular axis from the heavier to the lighter nucleus. The electronic factor $W_A$ is found from evaluating the matrix elements of the $\alpha \rho(r)$ operator in the molecular spinor basis [27]. The $^2\Sigma^+_{1/2}$ and $^2\Pi_{1/2}$ open-shell electronic states are two-fold degenerate, corresponding to the two possible projections of electronic angular momentum along $n$, i.e. $\Omega = |\pm \frac{1}{2}|$. When operating within this degenerate space, the operator $\frac{\kappa_{\text{NSD}}}{2} \alpha \rho(r)$ is equivalent to $W_A (n \times S')$ (Eq. (3)). Time-reversal symmetry ensures that only the matrix elements that are off-diagonal in $\Omega$ are non-vanishing. This symmetry rule is encapsulated within the effective operator $H^{\text{eff}}_A$ by the angular factor $(n \times S')$. Here the effective spin $S'$ generates rotations in the degenerate subspace analogously to the usual spin operator $S$ in a spin-1/2 system.

The calculations were carried out within the open-shell single determinant average-of-configuration Dirac-Hartree-Fock approach [28] and within the relativistic density functional theory [29], employing quaternion symmetry [30, 31]. A finite nucleus, modeled by the Gaussian charge distribution was used [32]. In the DFT calculations we used the Coulomb-attenuated B3LYP functional (CAMB3LYP*), the parameters of which were adjusted by Thierfelder et al. [33] to reproduce the PV energy shifts obtained using coupled cluster calculations (the adjusted parameters are $\alpha = 0.20$, $\beta = 0.12$, and $\mu = 0.90$). All the calculations were performed using the DIRAC12 program package [34].

| Atom | $Z$ | Basis Set |
|------|-----|-----------|
| N    | 7   | aug-cc-PVTZ |
| O    | 8   | aug-cc-PVTZ |
| F    | 9   | aug-cc-PVTZ |
| Mg   | 12  | aug-cc-PVTZ |
| Si   | 14  | aug-cc-PVTZ |
| Ca   | 20  | aug-cc-PVTZ |
| Sc   | 21  | 19s17p10d7f2g |
| Ti   | 22  | 21s16p10d7f2g |
| Zn   | 30  | 21s19p10d7f2g |
| Ge   | 32  | 20s20p11d8f2g |
| Br   | 35  | 21s20p10d10f1g |
| Sr   | 38  | 21s20p12d9f2g |
| Y    | 39  | 21s20p12d9f2g |
| Zr   | 40  | 21s20p12d9f2g |
| Cd   | 48  | 22s20p12d9f2g |
| Sn   | 50  | 21s21p12d9f2g |
| Ba   | 56  | 24s22p15d10f2g |
| La   | 57  | 24s22p14d10f2g |
| Yb   | 70  | 26s21p14d10f2g |
| Hf   | 72  | 25s22p16d10f2g |
| Hg   | 80  | 25s21p15d10f2g |
| Pb   | 82  | 25s22p16d10f2g |
| Ra   | 88  | 26s23p16d11f2g |
| Ac   | 89  | 26s24p16d11f2g |

* augmented by 2 high exponent $s$ and 4 high exponent $p$ functions.

For the lighter elements (N to Si), the aug-cc-pVTZ basis sets were used [35, 36], all in their uncontracted form, as it is important to have maximum flexibility of the wavefunction in the region close to the nucleus. For the rest of the atoms, we employed the Faegri’s dual family basis sets [37]. As a good description of the electronic wave function in the nuclear region is essential for obtaining reliable results for parity violating properties [38], we augmented the basis sets with high exponent $s$ and $p$ functions, which brings about an increase of around 10% in the calculated values of $W_A$. The basis sets were increased, both in the core and in the valence regions, to convergence with respect to the calculated $W_A$ constants. The final basis sets can be found in Table I.

Where available, experimental bond distances $R_e$ were used. For molecules where $R_e$ is not known experimentally we optimized the bond distance using the relativistic coupled cluster approach with single, double, and perturbative triple excitations, CCSD(T) [39]. To reduce the computational effort, we employed an infinite order two-component relativistic Hamiltonian obtained after the Barysz–Sadlej–Snijders (BSS) transformation of the Dirac Hamiltonian in a finite basis set [40, 41]. Our calculated $R_e$ are typically within 0.01 Å of the experimental values, where available.

In our previous work [25] we have examined and
compared various schemes for adding electron correlation to the Dirac–Hartree–Fock $W_A$ values, and core-polarization contributions to the DFT results. Here, we correct the calculated DHF and DFT $W_A$ for core polarization using a scaling parameter, $K_{CP}$. This parameter is obtained from atomic calculations as described in the following.

The main contribution to the matrix elements of the NSD interaction for the valence molecular electrons comes from short distances around the heavy nucleus, where the total molecular potential is spherically symmetric to very high precision, and the core of the heavy atom is practically unaffected by the presence of the second atom, justifying our use of the atomic model. The molecular orbitals of the valence electron can thus be expanded in this region, using spherical harmonics centered at the heavy nucleus,

$$|\psi_v\rangle = a|s_{1/2}\rangle + b|p_{1/2}\rangle + c|p_{3/2}\rangle + d|d_{3/2}\rangle \ldots$$  \hspace{1cm} (4)

Only $s_{1/2}$ and $p_{1/2}$ terms of this expansion give significant contribution to the matrix elements of the weak interaction. These functions can be considered as states of an atomic valence electron and are calculated using standard atomic techniques in two different approximations: one that includes electron correlation and another that does not.

The single electron DHF Hamiltonian is given by

$$\hat{H}_0 = c\alpha \cdot \mathbf{p} + (\beta - 1)c^2 - \frac{Z}{r} + V_c(r),$$ \hspace{1cm} (5)

where $\alpha$ and $\beta$ are the Dirac matrices and $V_c(r)$ is the self-consistent DHF potential due to atomic electrons.

The self-consistent DHF procedure is first performed for the closed shell ion, from which the valence electron is removed. Then the core potential $V_{\text{DHF}}^{N-N_c}$ is frozen and the valence $s_{1/2}$ and $p_{1/2}$ states are calculated by solving the DHF equation for the valence electron,

$$(\hat{H}_0 - \epsilon_v)|\psi_v\rangle = 0,$$ \hspace{1cm} (6)

where $\hat{H}_0$ is given by (5).

The core polarization can be understood as the change of the self-consistent DHF potential due to the effect of the extra term (the weak interaction operator $\hat{H}_A$) in the Hamiltonian. The inclusion of the core polarization in a self-consistent way is equivalent to the random-phase approximation (RPA, see, e.g. [22]). The change in the DHF potential is found by solving the RPA-type equations self-consistently for all states in the atomic core,

$$(\hat{H}_0 - \epsilon_c)\delta\psi_c = (\hat{H}_A + \delta V_A)\psi_c.$$ \hspace{1cm} (7)

Here, $\hat{H}_0$ is the DHF Hamiltonian [3], index $c$ enumerates the states in the core, $\delta\psi_c$ is the correction to the core state $c$ due to weak interaction $\hat{H}_A$, and $\delta V_A$ is the correction to the self-consistent core potential due to the change of all core functions. Once $\delta V_A$ is found, the core polarization can be included into a matrix element for valence states $v$ and $w$ via the redefinition of the weak interaction Hamiltonian,

$$\langle v|\hat{H}_A|w\rangle \rightarrow \langle v|\hat{H}_A + \delta V_A|w\rangle.$$ \hspace{1cm} (8)

We then obtain the scaling parameter for core-polarization effects, $K_{CP}$, from

$$K_{CP} = \frac{\langle \psi^{\text{DHF}}_{n_{s1/2}}|\hat{H}_A + \delta V_A|\psi^{\text{DHF}}_{n_{p_{1/2}}}\rangle}{\langle \psi^{\text{DHF}}_{n_{s1/2}}|\hat{H}_A|\psi^{\text{DHF}}_{n_{p_{1/2}}}\rangle}.$$ \hspace{1cm} (9)

It should be noted that for the group 14 fluorides we have only calculated the correlations between the valence electrons and the core; the correlations between the valence $ns$ and $np$ electrons are not included.

As the final recommended value for the $W_A$ parameter we take an average of $W_A(\text{DHF})K_{CP}$ and $W_A(\text{DFT})K_{CP}$. The estimate of the accuracy of the final results in our previous work [23] has shown that it is about 15% for the $\Sigma^+_1/2$ electronic state and 20-30% for the $^2\Pi_{1/2}$ state.

### III. Results and Discussion

Table II contains the $W_A$ constants obtained for neutral molecules, where other theoretical results are available. To the best of our knowledge this table sums up all the existing calculations of the $W_A$ parameter for neutral diatomic molecules. These systems were discussed in our earlier publication [23]; however our improved results presented here are are lower than the values shown in Ref. [25] due to the more accurate treatment of the finite nuclear size and a better treatment of the basis set. This decrease is only 5% for the lighter systems but up to 20% for the heaviest ones. The contribution of correlation on the DFT level to the calculated $W_A$ constants is very small, and for the majority of the molecules considered here it is less than 10%.

For MgBr, SrF, ZrN, BaF, LaO, YbF, HgF, and PbF a number of semiempirical calculations were performed [11, 16–18]. For the lighter systems our $W_A$ constants are about 10-20% lower than the semiempirical values, for HgF and PbF our values are higher. This discrepancy requires still some future attention and will be resolved only if a more accurate electron correlation treatment becomes available. There is already progress in this direction [19].

Our uncorrelated DHF values are in very good agreement with those from Refs. [19, 21, 23]. In particular, the recently published quasirelativistic two-component zero-order regular approximation (ZORA) HF $W_A$ constants for group 2 fluorides [23] do not differ by more than a few percent from the values obtained here. This shows that the performance of the ZORA approximation compared to the 4-component Dirac Hamiltonian is indeed very good for the properties studied here. Ref. [23] is
TABLE II. Internuclear distances $R_e$ (Å) (experimental, Ref. [43], unless referenced otherwise), core-polarization scaling parameters $K_{CP}$, the $P$-odd interaction constants $W_A$ (Hz) obtained using DHF and DFT methods, and the final recommended values, $W_A$(Final), compared to earlier results.

| $Z$ | $R_e$ (Å) | $K_{CP}$ | $W_A$ (Hz) Previous results | $W_A$ (Hz) Final | Method | Ref. |
|-----|-----------|----------|------------------------------|-----------------|--------|------|
|     |           |          | DHF | DFT |       |       |       |
| MgF | 12        | 1.750    | 1.2 | 3.84 | 4.36  | 4.92  |       |
| CaF | 20        | 1.967    | 1.3 | 8.03 | 8.23  | 10.6  |       |
| MgBr| 35        | 2.360    | 1.2 | 8.24 | 17.4  | 16.2  |       |
| SrF | 38        | 2.075    | 1.3 | 40.7 | 39.0  | 51.8  |       |
| ZrN | 40        | 1.696    | 1.2 | 60.0 | 54.0  | 68.5  |       |
| BaF | 56        | 2.162    | 1.3 | 112.9| 111.6 | 146.0 |       |
|     |           |          |     |     |       |       |       |
|     |           |          |     |     |       |       |       |
| LaO | 57        | 1.825    | 1.2 | 149.4| 146.0 | 180.2 |       |
| YbF | 70        | 2.016    | 1.2 | 466.5| 494.0 | 576.3 |       |
|     |           |          |     |     |       |       |       |
|     |           |          |     |     |       |       |       |
| HgF | 80        | 2.025    | 1.1 | 3024.7| 2724.5| 3162.1|       |
| PbF | 82        | 2.075    | 1.1 | -1139.9| -1167.6| -1269.1|       |
| RaF | 88        | 2.256    | 1.2 | 1363.9| 1371.4| 1641.2|       |

$^a$ Quasirelativistic two-component zero-order regular approximation
$^b$ B3LYP functional
$^c$ Fully relativistic restricted active space configuration interaction method.
$^d$ Relativistic effective core potential (RECP) combined with SCF
$^e$ RECP combined with SCF and an effective operator to account for core-valence correlations.
$^f$ RECP combined with restricted active space SCF approach and an effective operator to account for core-valence correlations.
$^g$ Scaled by a semiempirical parameter to estimate spin-polarization contribution
$^h$ CCSD(T), present calculations
$^i$ RECP combined with spin-orbit direct configuration interaction

also the only other publication where the DFT approach was used. The slightly larger (compared to the difference between the HF results) discrepancies between our DFT values and those from Ref. [23] can be attributed to a different choice of functional.

Our final results, corrected for the core polarization contribution, can be compared to the values obtained in Refs. [20, 23, 44]. In Refs. [20, 44], the authors correct for the core polarization contribution by introducing an effective operator (EO), formed in the framework of the atomic many-body perturbation theory. This method was applied to the BaF and the YbF molecules, increasing the calculated $W_A$ constant by 70% and by 30%, respectively, compared to the SCF values. The second attempt to correct for the core polarization contribution is from Ref. [23], where a scaling parameter derived from a semiempirical molecular model of Kozlov [46] was applied to the HF $W_A$ constants of BaF, YbF, and RaF, also increasing their magnitude. The results obtained using the two approaches are in very good agreement with each other. Our final values are lower by about 20% compared to those of Refs. [20, 23, 44], as the magnitude of the scaling parameters used in this work is 1.1-1.3. Overall, our results are in good agreement with the majority of the previous investigations.

Table III contains the recommended $W_A$ parameters.
TABLE III. Internuclear distances $R_e$ (Å) (experimental, Ref. 33, unless referenced otherwise), core-polarization scaling parameters $K_{CP}$, the $P$-odd interaction constants $W_A$ (Hz) obtained using DHF and DFT, and the final recommended values, $W_A$(Final) for neutral diatomic molecules.

| $Z$ | $R_e$ (Å) | $K_{CP}$ | $W_A$ (Hz) | DHF | DFT | Final |
|-----|-----------|----------|------------|------|-----|-------|
|     |           |          |            |      |     |       |
| Group 3 oxides ($^2\Sigma_{1/2}$) |           |          |            |      |     |       |
| ScO | 21        | 1.668    | 1.2        | 11.5 | 10.2| 13.0  |
| YO  | 39        | 1.790    | 1.2        | 54.9 | 53.6| 65.1  |
| LaO | 57        | 1.825    | 1.2        | 150.6| 147.8| 179.0 |
| AcO | 89        | 1.962    | 1.2        | 2007.9| 1973.5| 2388.9 |
| Group 4 nitrides ($^2\Sigma_{1/2}$) |           |          |            |      |     |       |
| TiN | 22        | 1.582    | 1.2        | 11.6 | 10.2| 13.1  |
| ZrN | 40        | 1.696    | 1.2        | 59.9 | 53.9| 68.3  |
| HfN | 72        | 1.736    | 1.2        | 772.2| 715.1| 892.4 |
| Group 12 fluorides ($^2\Sigma_{1/2}$) |           |          |            |      |     |       |
| ZnF | 30        | 1.766    | 1.1        | 52.1 | 57.4| 60.3  |
| CdF | 48        | 1.991    | 1.1        | 220.3| 227.4| 246.3 |
| HgF | 80        | 2.025    | 1.1        | 3024.7| 2724.5| 3162.1 |
| Group 14 fluorides ($^2\Pi_{1/2}$) |           |          |            |      |     |       |
| SiF | 14        | 1.601    | 1.1        | −0.04|−0.05|−0.05 |
| GeF | 32        | 1.745    | 1.1        | −2.74|−3.17|−3.25 |
| SnF | 50        | 1.944    | 1.1        | −30.0|−34.1|−35.3 |
| PbF | 82        | 2.078    | 1.1        | −1139.9|−1167.6|−1269.1 |

$^a$ CCSD(T), present calculations  
$^b$ Ref. 27

TABLE IV. The $Z$-exponent $a$ and the prefactor $b$, derived from $\log\left(\frac{W_A}{R_W}\right)$ as a function of $\log(Z)$.

|            | $a$     | $\log(b)$ |
|------------|---------|-----------|
| DHF        | DFT     | Final     |
| Group 2 fluorides | 1.80   | 1.74     | 1.77     | −1.45 | −1.35 | −1.30     |
| Group 3 oxides     | 1.98   | 2.05     | 2.01     | −1.65 | −1.78 | −1.63     |
| Group 4 nitrides     | 2.35   | 2.39     | 2.37     | −2.18 | −2.30 | −2.16     |
| Group 12 fluorides    | 2.49   | 2.28     | 2.38     | −2.12 | −1.77 | −1.90     |
| Group 14 fluorides    | 4.67   | 4.57     | 4.61     | −6.78 | −6.56 | −6.61     |

$R_W = \frac{2\gamma + 1}{3} \left( \frac{a_B}{2Zr_0A^{1/3}} \right)^{2-2\gamma} \frac{4}{\Gamma(2\gamma + 1)^2}$ (10)

In Eq. (10), $a_B$ is the Bohr radius, $r_0 = 1.2 \times 10^{-15}$ m, and $\alpha$ is the fine-structure constant. In Fig. 1, we plot $\log\left(\frac{W_A}{R_W}\right)$ as a function of $\log(Z)$ for the five groups of dimers studied here. A linear fit for each of the groups provides us with the $Z$-exponent $a$ and prefactor $b$ for $|W_A| = bR_WZ^a$, listed in Table IV for the DHF, DFT, and the final results. The $a$ and $b$ parameters are in good agreement for the DHF and the DFT approaches. For group 2 fluorides and group 3 oxides the scaling is, indeed, close to $Z^2$, as suggested by Eq. (10). For group 4 nitrides and group 12 fluorides the $Z$-dependence is much more advantageous, of $Z^4$, due to the filling of the lower lying $d$-shell, which expands relativistically and thus increases the effective nuclear charge, leading to an enhancement of relativistic and PV effects, and an increase of $W_A$. Moreover, even though the group 3 oxides and group 4 nitrides are iso-electronic, nitrogen is more electropositive than oxygen, thus increasing the electron density at the metal atom. This shows the subtle interplay of electronic effects in these molecules which should be further studied.

In the case of group 14 fluorides, the ground state is $^2\Pi_{1/2}$, for which the $W_A$ parameter vanishes in the non-relativistic limit, since in this limit it does not contain the s-wave electronic orbital and can not provide the matrix element $\langle s_{1/2}\alpha\rho(r)|p_{1/2}\rangle$. The effect appears due to the mixing of the $^2\Sigma_{1/2}$ and $^2\Pi_{1/2}$ electronic states by the spin-orbit interaction, which obviously increases with increasing nuclear charge, and gives an extra factor of $Z^2\alpha^2$ in the $Z$-dependence of $W_A$, as seen in Table IV. However, in this case the prefactor $b$ is four orders of magnitude smaller. Nevertheless, it shows that such molecules should not be discarded for the successful measurement of the anapole moment.

![FIG. 1. (color online) Scaling of $\log\left(\frac{W_A}{R_W}\right)$ with $\log(Z)$ for the investigated molecules.](image-url)
IV. CONCLUSIONS

We have obtained the much improved $W_A$ parameters for diatomic molecules from relativistic HF and DFT calculations using corrections for core polarization effects. The scaling of the $W_A$ parameter with the nuclear charge $Z$ was examined in different groups and found to be advantageous in group 4 nitrides and group 12 fluorides. Some of the heavier molecules, such as HgF and PbF, should be excellent candidates for future NSD PV measurements. The accurate inclusion of electron correlation within a fully relativistic framework in the calculations of the $W_A$ parameters, which still remains a challenge, will be the focus of our future work.

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