

Constraints on New Vector Boson Mediated Electron-Nucleus Interactions from Spectroscopy Data of Polar Diatomic Molecules

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A measurement of parity violation in the hyperfine structure of $^{138}\text{Ba}^{19}\text{F}$ [E. Altuntaş *et al.* *Phys. Rev. Lett.* **120**, 142501 (2018)] is reinterpreted with electronic structure calculations in terms of beyond standard model vector boson mediated electron-nucleus interactions. Our results set constraints on previously unexplored, new boson mediated axial vector-vector nucleus-electron interactions. Similar bounds are obtained by analyzing the atomic parity violation experiment with ^{133}Cs . Moreover, we show that future experiments with cold heavy diatomic molecules like ^{137}BaF or ^{225}RaF can improve the present sensitivity to axial vector-vector nucleus-electron and nucleon-nucleus interactions by at least 2 orders of magnitude for large boson masses.

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Introduction—The proposal to test for parity (P) violation (PV) in weak interactions by Lee and Yang [1] and its rapid experimental realization by Wu *et al.* [2] changed paradigms in the view on discrete symmetries in fundamental physical processes. In recent years, new bosons mediating parity-violating interactions have been proposed as promising dark-matter candidates [3–8]. Of these, the spin-1 Z' boson is of particular interest because it is predicted by various extensions of the standard model (SM) of particle physics [9–12] and its role as a possible link between matter and dark matter [13,14]. Moreover, parity-violating interactions have been discussed in the context of the proposed 17 MeV boson (X17) [15–18].

Precision spectroscopy of heavy atoms such as Cs [19], Yb [20,21], Tl [22], and Dy [23,24] serves as a powerful tool to test electroweak PV within the SM as well as PV due to new spin-1 bosons beyond the SM (BSM) [25]. In atoms, nuclear spin-independent effects—or more general axial vector (A)-vector (V) electron (e)-nucleus (N) interactions (AV-eN) dominate—while nuclear spin-dependent PV (NSDPV) effects are typically suppressed. Three types of interactions contribute to NSDPV: (i) AV nucleus-electron interactions (AV-Ne), (ii) hyperfine interaction

induced AV-eN interactions, and (iii) electromagnetic interactions of electrons with weak nuclear moments like the anapole moment. The latter arise primarily from AV proton (p) or neutron (n)-nucleus (N) interactions, AV-(n,p)N. Dzuba *et al.* extracted the currently best bounds on new boson mediated spin-independent AV-eN interactions from the 6s-7s E1 transition in ^{133}Cs . The corresponding coupling constant was constrained to be $|g_e^A g_N^V| < 3.9 \times 10^{-8} M^2 c^4 / \text{GeV}^2$ for $M \rightarrow \infty$ and $|g_e^A g_N^V| < 3.1 \times 10^{-14}$ for $M \rightarrow 0$ [25]. By comparing NSDPV effects in different hyperfine components of this forbidden transition, they inferred the best constraints on AV-pN interactions to be $|g_p^A g_N^V| < 2.3 \times 10^{-5} M^2 c^4 / \text{GeV}^2$ for $M \rightarrow \infty$ and $|g_p^A g_N^V| < 6.0 \times 10^{-8}$ for $M \rightarrow 0$. AV-Ne interactions were not discussed in Ref. [25].

In contrast to atomic PV experiments, nuclear spin-independent AV-eN interactions in polar diatomic molecules are typically suppressed, making these systems particularly sensitive to NSDPV processes [26–28]. NSDPV manifests in these molecules as a mixing of Λ - or Ω -doublet states, which are connected by space- and time-parity inversion. In the molecular hyperfine structure, the effective PV spin-rotation (sr) Hamiltonian is [28]

$$\hat{H}_{\text{PV,sr}} = k_A W_a \vec{\lambda} \times \vec{S}' \cdot \vec{I}, \quad (1)$$

where $\vec{\lambda}$ is the unit vector pointing from the heavy to the light nucleus, $\vec{S}'$ is the effective electron spin, and $\vec{I}$ is the nuclear spin. In our notation, $\vec{S}'$ and $\vec{I}$ do not contain $\hbar$. Here $W_a = \langle \Omega | \hat{H}_{\text{NSDPV}} | -\Omega \rangle / \Omega$, where $\hat{H}_{\text{NSDPV}}$ is the NSDPV Hamiltonian. $k_A = k_a + k_{\text{AV}} + k_{\text{hf}}$ is a nuclear

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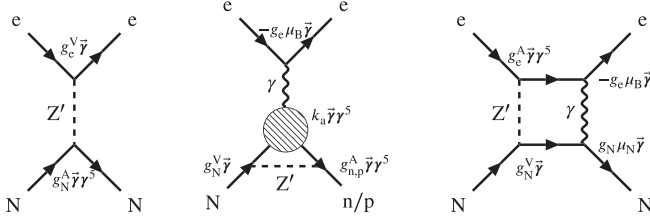


FIG. 1. Feynman diagrams illustrating contributions to parity-violating mixing in the BaF experiment from new Z' -like bosons. The left diagram shows the direct nuclear spin-dependent AV-Ne interaction between the nucleus (N) and the electron (e) mediated by a new boson. The middle diagram shows the electromagnetic interaction (mediated by a photon γ) between the electron and the nuclear anapole moment k_a , represented by the hatched vertex and arising from AV-(n,p)N interactions. The right diagram shows a second-order process in which the electron couples to the nucleus through two interactions: a new boson mediated AV-eN interaction and the electromagnetic hyperfine interaction. The electron and nuclear g factors are denoted by g_e and g_N , respectively, and μ_B and μ_N are the Bohr and nuclear magnetons.

structure dependent parameter containing contributions from the nuclear anapole moment (a), electroweak AV-Ne, and hyperfine (hf) induced AV-eN current interactions. The effective constant k_{hf} depends on the electronic structure.

Experiments have been proposed for a variety of molecular systems (see reviews [28–32] and references therein, as well as Refs. [33–37]). In 2018, an experiment with ^{138}BaF ($I_{\text{Ba}} = 0$) achieved sufficient spectral resolution that, if repeated with ^{137}BaF , would allow detection of NSDPV contributions from the ^{137}Ba nucleus [38]. More recently, further improvements in experimental precision have been proposed using Penning-trapped molecular ions [39].

In this Letter, we perform molecular density-functional-theory calculations to extract constraints on previously unexplored new boson mediated AV-Ne interactions from the PV experiment with $^{138}\text{Ba}^{19}\text{F}$ [38]. In addition, we extract comparable constraints from a reanalysis of the PV effect on hyperfine components of the forbidden atomic transition in ^{133}Cs . To the best of our knowledge, prior experimental constraints were limited to AV-ne and AV-pe interactions and applied only to new boson masses below $10^{-4} \text{ eV}/c^2$ [40,41] (see also Ref. [7] for a review). Our results extend the sensitivity to the subatomic scale ($M \sim 10^5 \text{ eV}/c^2$). Finally, we demonstrate that PV experiments with polar diatomic molecules have the potential to improve the present sensitivity to AV-Ne and AV-(n,p)N by several orders of magnitude.

Theory—A new spin-1 boson would modify the PV matrix element $k_A W_a$ via the AV interactions visualized in Fig. 1 by

$$\Delta k_{A,K} W_{a,K} = g_{N,K}^A g_e^V W_{\text{AV-Ne},K} + g_{N,K}^V g_e^A W_{\text{AV-eN},K} + g_{n,p}^A g_N^V k_{a,\text{AV-(n,p)N},K} \frac{M^2 c e}{\epsilon_0 \hbar^3} \lim_{M \rightarrow \infty} W_{\text{AV-Ne},K} \quad (2)$$

for every spin-carrying nucleus K in the molecule. g_i^A and g_i^V are the axial vector and vector coupling constants of particle i , where i is the electron (e), the nucleus (N), or a single nucleon (n,p). For nuclei, the coupling constants are approximately given as effective coupling constants $g_{N,K}^A \approx \langle \sigma \rangle_{p,K} g_p^A + \langle \sigma \rangle_{n,K} g_n^A$ and $g_{N,K}^V \approx (Z_K g_p^V + N_K g_n^V) / (Z_K + N_K)$, respectively. Here, $\langle \sigma \rangle_{p,K}$ and $\langle \sigma \rangle_{n,K}$ denote the average proton and neutron spin contributions, while Z_K and N_K are the proton, neutron numbers of nucleus K , respectively.

The three contributions stemming from AV-Ne, AV-(n,p)N, and AV-eN interactions arise—in analogy to the weak interactions—as mixing of Ω and $-\Omega$ states. The electronic structure coefficients W are computed in close analogy to SM PV matrix elements as

$$W_{\text{AV-Ne}} = \langle \Omega | \hat{H}_{\text{AV-Ne}} | -\Omega \rangle / \Omega, \quad (3)$$

$$W_{\text{AV-eN}} = \sum_{a \neq \Omega} \frac{\langle \Omega | \hat{H}_{\text{hf}} | a \rangle \langle a | \hat{H}_{\text{AV-eN}} | -\Omega \rangle}{\Omega(E_\Omega - E_a)} + \sum_{a \neq \Omega} \frac{\langle \Omega | \hat{H}_{\text{AV-eN}} | a \rangle \langle a | \hat{H}_{\text{hf}} | -\Omega \rangle}{\Omega(E_\Omega - E_a)}, \quad (4)$$

where $W_{\text{AV-eN}}$ is represented here in second order perturbation theory as a sum over all electronic states $|a\rangle$ with energy E_a except the $|\Omega\rangle$ state with energy E_Ω . $\hat{H}_{\text{hf}}$ is the electromagnetic hyperfine interaction operator. For more details see Supplemental Material [42]. A new spin-1 boson can couple a valence nucleon to the remaining nucleons and contribute to the nuclear anapole moment of nucleus K as [25]

$$k_{a,\text{AV-(n,p)N},K} = \begin{cases} \frac{18eR_K(Z_K + N_K)\mu_{n,p}}{25c} & Mc/\hbar \ll 1/R_K \\ \frac{9e\hbar^2(Z_K + N_K)\mu_{n,p}}{5c^3 M^2 R_K} & Mc/\hbar \gg 1/R_K, \end{cases} \quad (5)$$

where c is the speed of light in vacuum, e is the elementary electric charge, and $\hbar$ is the reduced Planck constant. Here, $R_K \approx 1.2 \text{ fm}(Z_K + N_K)^{1/3}$ denotes the nuclear charge radius, $\mu_{n,p}$ is the magnetic dipole moment of the valence neutron or proton ($\mu_p = 2.79\mu_N$, and $\mu_n = -1.91\mu_N$) in nuclear magnetons $\mu_N = e\hbar/(2m_p)$, with m_p being the proton mass.

Assuming the nucleons to be nonrelativistic and having a density distribution $\rho_K(\vec{r}_i)$, the PV electron-nucleus interaction operators are [25,72]

$$\hat{H}_{\text{AV-eN}} = \frac{\hbar c}{4\pi} \sum_i^{N_{\text{elec}}} \sum_K^{N_{\text{nuc}}} (Z_K + N_K) \gamma_i^5 V_{Y,K}(\vec{r}_i), \quad (6)$$

$$\hat{H}_{\text{AV-Ne}} = \frac{\hbar c}{4\pi} \sum_i^{N_{\text{elec}}} \sum_K^{N_{\text{nuc}}} \vec{l}_K \cdot \vec{\alpha}_i V_{Y,K}(\vec{r}_i), \quad (7)$$

where the Yukawa-like electron-nucleus potential is

$$V_{Y,K}(\vec{r}_i) = \int d^3r' \rho_K(\vec{r}') \frac{\exp(-Mc/\hbar|\vec{r}_i - \vec{r}_K - \vec{r}'|)}{|\vec{r}_i - \vec{r}_K - \vec{r}'|}. \quad (8)$$

Here, $\vec{r}_i$ denotes the position operator of electron i , with $r_{iK} = |\vec{r}_i - \vec{r}_K|$, and the sums run over all electrons i and nuclei K . $\vec{r}_K$ and $\vec{I}_K$ are the position and spin of nucleus K . The Dirac matrices $\vec{\alpha}, \gamma^5$ are used in standard notation and are defined in Supplemental Material [42]. In the following, we assume a pointlike nucleus, for which the Yukawa-like potential reduces to $V_{Y,A}(\vec{r}_i) = \exp(-Mc/\hbar r_{iA})/r_{iA}$. To compute the sensitivity to AV-(n,p)N interactions, we assume a finite nucleus described by a spherical Gaussian charge density distribution. In this case, the Yukawa-like potential reduces in the limit of large boson masses to $\lim_{M \rightarrow \infty} V_{Y,K} = \hbar^2 4\pi \rho_K(r_{iK})/(Mc)^2$. For heavy nuclei, finite nuclear size effects are expected to be sizable. In Supplemental Material [42], we provide a comparison between the pointlike nuclear model and finite nuclear model for the limits $M \rightarrow \infty$ and $M \rightarrow 0$. This comparison shows that the resulting errors are negligible for $M \rightarrow 0$, whereas errors are sizeable for $M \rightarrow \infty$, with the largest relative error ($\sim 40\%$) found for AV-eN interactions in RaF. This does not significantly affect the discussion and figures presented below.

Molecular density functional theory calculations—In order to obtain constraints on new boson mediated interactions from the $^{138}\text{Ba}^{19}\text{F}$ experiment, as well as from experiments with ^{137}BaF and isotopologues of RaF and SiO^+ , we compute electronic enhancement factors $W_{\text{AV-eN}}$ and $W_{\text{AV-Ne}}$ using molecular density functional theory employing a quasirelativistic two-component Hamiltonian within zeroth order regular approximation (ZORA). All calculations were carried out with the program package [49,50], which is based on Turbomole [51]. We employed the same methodology as in Ref. [52]: a hybrid local density approximation with 50% Fock exchange by Becke (BHandH) [53–55,73], together with a large atom-centered Gaussian basis set by Dyllal (dyall.cv4z) [56], augmented with additional tight s- and p-type functions as described in Supplemental Material [42]. This approach shows excellent agreement with relativistic coupled cluster calculations of other symmetry violating properties [52]. Further computational details are provided in Supplemental Material [42].

At this level of theory, we accurately reproduce relativistic coupled-cluster results for the electroweak PV matrix element arising from the anapole moment in ^{137}Ba , $|W_a|$, obtaining 149 Hz compared to 147.7 Hz reported in Ref. [74]. Similarly excellent agreement is found for $|W_a|$ in ^{225}RaF , where our result (1731 Hz) closely matches sophisticated coupled-cluster calculations (1694 Hz) [75,76]. For $^{29}\text{SiO}^+$, our computed electroweak matrix element (15 Hz) is in reasonable agreement with four-component coupled-cluster

calculations (13 Hz) [39]. We provide a list of matrix elements contributing to $\Delta k_{A,K} W_{a,K}$ for different boson masses for all studied molecules in Supplemental Material [42].

Constraints from the $^{138}\text{Ba}^{19}\text{F}$ experiment—To extract constraints on new boson mediated interactions, experimental uncertainties and uncertainties in the SM predictions must be combined with calculations of the BSM coupling matrix elements. We compute the SM-PV matrix element to be $k_{A,^{19}\text{F}}|W_{a,^{19}\text{F}}| = 0.014 \hbar \text{ Hz } k_{A,^{19}\text{F}}$. Our predicted value of W_a is of the same order of magnitude as the estimate reported in Ref. [38]. Using the estimate $k_{A,^{19}\text{F}} \approx -0.08$ [33,38,57], the resulting SM contribution $k_A W_a$ is more than 2 orders of magnitude smaller than the current experimental uncertainty of $\Delta\nu = 0.7 \text{ Hz}$ reported in Ref. [38]. Therefore, at the current level of experimental precision, nuclear-theory uncertainties do not limit the extracted bounds. To demonstrate this, we present in Supplemental Material [42] a table illustrating the impact of hypothetical nuclear-theory uncertainties of 100%, 400%, and 1000%. We emphasize that nuclear-structure uncertainties will become essential once experimental sensitivities reach the mHz level. The resulting constraints on new spin-1 boson AV-Ne, AV-eN, and AV-pN interactions are shown as the red regions in Fig. 2.

To the best of our knowledge, this is the first direct constraint for AV-Ne interactions [shown in Fig. 2(a)]. For comparison, we extracted constraints on AV-Ne interactions from the atomic Cs PV experiment by relating the uncertainty in $k_{A,^{133}\text{Cs}}$ from Refs. [25,78] $\Delta k_{A,^{133}\text{Cs}} \approx 0.236$ to AV-Ne interactions under the assumption that the new boson contribution to the nuclear anapole moment is zero. We note that the value $\Delta k_{A,^{133}\text{Cs}}$ was derived under the assumption that the nuclear theory uncertainty would be only 30% [25,78]. As the actual uncertainty of the anapole moment calculation of Cs might be larger [74], the constraints from Cs are probably rather optimistic. In this work, the influence of a larger uncertainty on the constraints is mild: for example a 100% uncertainty would weaken bounds roughly by a factor of two which is hardly visible in Fig. 2. A systematic comparison is provided in Supplemental Material [42] for several representative theoretical uncertainty levels. For $M > \text{MeV}/c^2$, the ratio between the electroweak NSDPV matrix element and the new boson NSDPV matrix element is $(\hbar^3 \sqrt{2} g_e^V g_N^A)/(4\pi G_F c M^2) \approx 9.62 \times 10^{21} g_e^V g_N^A \text{ eV}^2/(M^2 c^4)$. In analogy to new boson mediated AV-eN interactions in Cs [25], we assume that the limit $M \rightarrow 0$ is reached for masses $M \lesssim 200 \text{ keV}/c^2$. In this limit, we obtain $\lim_{M \rightarrow 0} \Delta k_A \approx 2.4 \times 10^{11} g_e^V g_N^A$. The obtained constraints are shown in Fig. 2(a) as the orange area. These Cs constraints are about 1 order of magnitude weaker than constraints from $^{138}\text{Ba}^{19}\text{F}$ for $M < \text{keV}$ and are not more than 1 order of magnitude stronger for $M > 100 \text{ keV}$, even though the nuclear charge number of Cs is six times larger than that of F. The fact that the current experimental precision in $^{138}\text{Ba}^{19}\text{F}$ is not limited by

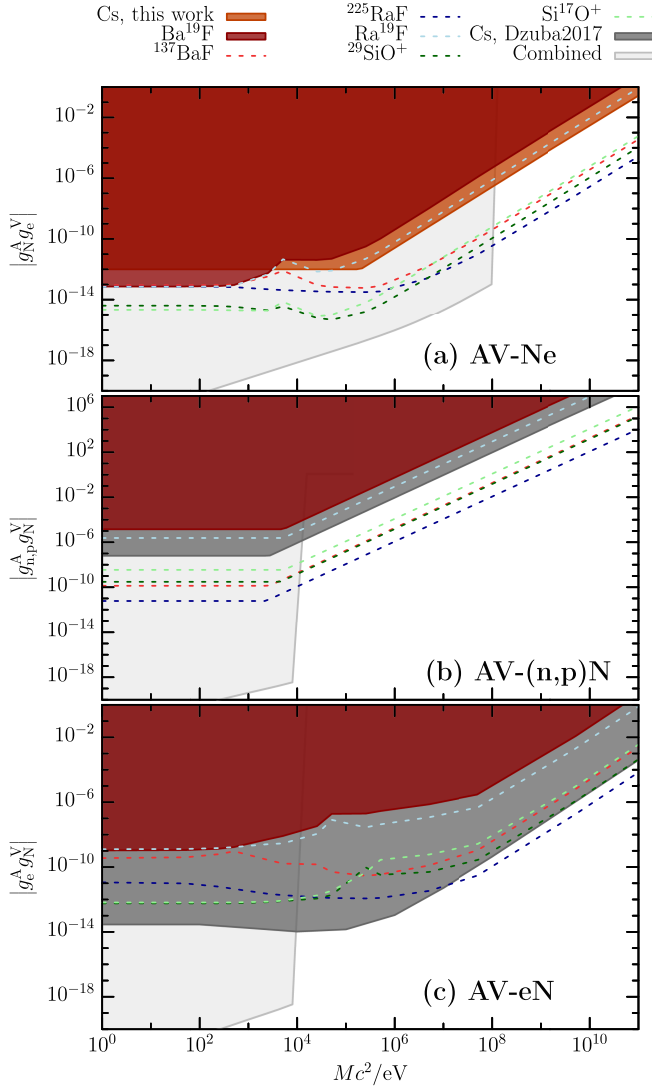


FIG. 2. Constraints (solid lines) and projected sensitivities (dashed lines) on new boson mediated (a) AV-Ne interactions, (b) AV-(n,p)N interactions, and (c) AV-eN interactions inferred from PV studies of atoms and diatomic molecules. Results of this work from the $^{138}\text{Ba}^{19}\text{F}$ and Cs PV measurements, as well as projections of future experiments with the diatomic molecules BaF, RaF, and SiO^+ , are shown. Constraints on AV-(n,p)N and AV-eN interactions are compared to constraints from an atomic PV analysis of Cs obtained in Ref. [25]. For comparison, combined constraints derived from astrophysical bounds on g_N^V [58], g_N^A [59] and laboratory bounds on g_e^V [60], g_e^A [61], g_p^A [62] are shown (for discussion see Refs. [7,77]). The nucleus which interacts with electrons via a new boson is indicated by its explicit mass number. Excluded regions are shown as filled areas, while projected sensitivities are shown as dashed lines. The projections do *not* include the theoretical nuclear-structure uncertainty in order to allow an unbiased comparison of electronic structure sensitivities. Modified plots including a representative nuclear-structure uncertainty of 100% are provided in Supplemental Material [42]. There, the projected limits for ^{137}BaF and SiO^+ are weakened by more than 1 order of magnitude, while those for ^{225}RaF are weakened by more than 2 orders of magnitude.

nuclear theory (in contrast to Cs) highlights the advantage of molecules over atoms for the detection of AV-Ne type interactions.

Note, that constraints on the coupling strength of new vector boson mediated interactions can be obtained from combining bounds (light gray filled area) on individual coupling strength g_e^V [60], g_e^A [61], g_p^A [62]. However, these combined bounds are model dependent and, therefore, PV experiments with atoms and molecules provide complementary information.

In Figs. 2(b) and 2(c), we compare the bounds obtained in this work with existing constraints on AV-(n,p)N and AV-eN interactions, shown as gray area. There also exist constraints on AV-e(n,p) interactions [21], but these are weaker by a few orders of magnitude compared to the constraints on AV-eN [25]. The $^{138}\text{Ba}^{19}\text{F}$ system is only slightly less sensitive to AV-(n,p)N interactions than the Cs experiment [25]. As expected from the generally lower sensitivity of $|\Omega\rangle$ states to nuclear spin-independent PV, discussed in the introduction, the $^{138}\text{Ba}^{19}\text{F}$ experiment is less sensitive to AV-eN interaction than atomic PV experiments [25].

The sensitivity of the BaF molecular experiments can be improved in a straightforward manner [33,38]. Assuming that the experiment were performed with $^{137}\text{Ba}^{18}\text{F}$, we find [bright red line in Figs. 2(a) and 2(b)] that the sensitivity to AV-eN and AV-Ne interactions would improve by 1–5 orders of magnitude, while the sensitivity to AV-(n,p)N interactions would be enhanced by about four orders of magnitude. We note here that future experiments employing vibrational spectroscopy of chiral molecules may be more sensitive to AV-(n,p)N interactions for boson masses $M < 10^4 \text{ eV}/c^2$ [79].

It has to be emphasized that the electroweak P -odd effect of an odd Ba nucleus would overshadow the new boson effect, and that the extraction of BSM physics will rely on accurate predictions from molecular and nuclear theory. Whereas the accuracy of molecular calculations is currently at the level of 1.5% for BaF [74], accurate nuclear structure calculations are lacking. Assuming an uncertainty of $\sim 30\%$ in the nuclear anapole moment calculation of ^{137}Ba , as adopted for ^{133}Cs [78] or even $\sim 100\%$, the uncertainty in $\Delta k_A W_a$ for ^{137}BaF may increase roughly to $\sim 3 \text{ Hz}$ or to $\sim 10 \text{ Hz}$, respectively, i.e., by a factor of 4 or 13. Here, we have coarsely estimated the size of the nuclear anapole moment as [57,63] $k_a \sim 1.15 \times 10^{-3} g_n \mu_n A^{2/3} (I + 1/2) / (I + 1) \leq 0.07$, where $g_n = 0.9 \pm 0.6$ [64]. However, we are confident that a first measurement of PV in BaF will motivate improved calculations of nuclear anapole moments. The different dependences on Z and A of SM and BSM contributions arising from the AV-eN and AV-Ne interactions to $k_A W_a$ can facilitate the disentanglement of SM-PV and BSM-PV contributions through comparisons among different BaF isotopologues ($^{130-141}\text{Ba}$). Disentangling anapole-moment contributions, however, requires complementary

measurements in other Ba-containing molecules or in Ba atoms using the same Ba isotope. Finally, the experimental uncertainty in BaF is expected to be further reduced by direct laser-cooling [80], which has recently been proposed for several isotopologues [81].

Projected sensitivity of PV experiments with other diatomic molecules—An experiment with RaF is expected to be more than 1 order of magnitude more sensitivity to electroweak PV effect than the BaF experiment [34,75,82], and ongoing experimental efforts promise the realization of an RaF PV experiment in the near future [76,83,84]. Radium possesses a long chain of isotopes with a half-life above one second, which renders precision spectroscopy of different RaF isotopologues particularly promising for separating SM-PV and BSM-PV [83,84]. For comparison with BaF, we assume the experimental sensitivity of the emerging RaF experiment to be equivalent to that of the BaF PV experiment [38] ($\Delta\nu = 0.7$ Hz). We neglect a possible uncertainty associated with nuclear anapole-moment calculations, which—under same assumptions as discussed for Cs and BaF above—would amount to $\Delta k_A W_a \sim 40$ Hz. The omission of nuclear-structure uncertainties in the projections is not meant to suggest that they are negligible, but solely to isolate the relative electronic-structure sensitivities of different systems. Including such an uncertainty would reduce the projected sensitivity of RaF by no more than 2 orders of magnitude as discussed in Supplemental Material [42]. The projected sensitivities for RaF are shown as blue lines in Fig. 2. The RaF PV experiment is planned to be performed with ^{225}Ra . For comparison, we also provide the projected BSM-PV sensitivity for a hypothetical experiment probing the ^{19}F nucleus. We find that Ra^{19}F is slightly more sensitive to PV than Ba^{19}F for masses $M > 10^4$ eV/ c^2 . RaF experiments with nonzero-spin Ra nuclei could improve the sensitivity of the BaF experiments to AV-Ne interactions by up to 1 order of magnitude and to AV-(n,p)N interactions by roughly 2 orders of magnitude. Moreover, an equally large improvement of the BaF experiment is expected for AV-eN interactions. This may allow to improve the sensitivity of PV experiments to AV-eN interactions for masses $M > 10^7$ eV/ c^2 . Finally, we note that the experimental resolution in RaF may be improved through direct laser cooling, which would play a more important role than in BaF owing to generally smaller numbers of molecules [34,76,85,86].

In contrast to experiments that aim to measure electroweak PV, studies of PV induced by new bosons benefit from lighter molecules, which exhibit smaller SM-PV effects and may therefore be particularly interesting for searches for new bosons with masses $M < 10$ keV. Recently, systems with light elements, such as MgCN or SiO^+ , have been discussed as candidates for electroweak PV experiments in a Penning trap [39,87]. The short-term precision of a PV experiment with SiO^+ has been estimated

to be limited by a statistical uncertainty of approximately 5% in the PV matrix-element, which amounts to about ~ 0.02 Hz [39]. For the purpose of a fair comparison and to illustrate the relative potential, the projections shown in Fig. 2 are extracted using our calculations without including the theory uncertainty. A nuclear theory uncertainty of 100% would weaken the projected constraints by roughly one order of magnitude (further details are provided in Supplemental Material [42]). These systems are competitive with upcoming experiments with ^{225}RaF or ^{137}BaF . Assuming that the uncertainty of calculations of the anapole moment would be considerably smaller than 30%, heavier molecules would exhibit substantially larger sensitivity to AV-(n,p)N interactions, as well as to AV-Ne and AV-eN interactions, for $M > 10^4$ eV/ c^2 . In contrast, for $M < 10^4$ eV/ c^2 , the projected sensitivity of SiO^+ to AV-Ne and AV-eN is more than 1 order of magnitude stronger than that obtained for ^{225}RaF or ^{137}BaF , even if the uncertainty of nuclear structure theory could be ignored. However, for assumed experimental uncertainties, atomic experiments remain one to two orders of magnitude more sensitive to AV-eN interactions for $M < 10^4$ eV/ c^2 .

Finally, we note that, in order to extract rigorous bounds on new bosons, all possible sources contributing to an observed PV effect must ultimately be considered simultaneously, i.e., AV-Ne, AV-eN and AV-(n,p)N interactions within the SM and beyond. This requires at least four complementary experiments, which must be analyzed within a multivariate framework similar to that employed in studies of CP violation beyond the SM [52,88,89]. We therefore regard the complementarity of molecular PV experiments with atomic experiments as a crucial ingredient for future searches for BSM Z' -like bosons.

Conclusion—We have analyzed PV experiments with diatomic molecules in terms of their sensitivity to new spin-1 bosons. Performing density-functional-theory calculations of new boson mediated PV electron–nucleus interactions in $^{138}\text{Ba}^{19}\text{F}$, we set constraints on previously unexplored AV-Ne interactions, as shown in Fig. 2(a). Comparable constraints are obtained from a reanalysis of the ^{133}Cs atomic PV experiment, which in contrast depend on nuclear theory uncertainties. Furthermore, by calculating new spin-1 boson interactions in the diatomic molecules ^{137}BaF , RaF, and SiO^+ , we demonstrate that upcoming PV experiments with diatomic molecules can improve the current sensitivity to AV-Ne and AV-(n,p)N interactions by at least 2 orders of magnitude, assuming state-of-the-art experimental resolution. Exploiting sensitivities beyond this level will likely be limited by uncertainties in nuclear anapole moment calculations.

The broad potential of molecular systems for probing NSDPV, is reflected in recent developments, including indirect measurements of NSDPV via PV nuclear spin–spin couplings in TIF [90] and nuclear magnetic resonance experiments with chiral molecules [91]. In addition,

vibrational spectroscopy of chiral molecules—a prospective direct probe of new vector bosons [92,93]—has been shown to provide sensitivity to AV-eN interactions that is competitive to atomic PV experiments [79].

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Data availability—The data that support the findings of this article are openly available [95], embargo periods may apply.

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