A Program to Study Nuclear Spin-Dependent Parity Non-Conservation Using Simple Molecules

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The effects of nuclear spin-dependent parity nonconservation (NSD-PNC), which are of relevance in both nuclear and particle physics, can be dramatically enhanced in diatomic molecules. Here we outline a new method to investigate these effects based on laser and RF spectroscopy of the closely spaced hyperfine/rotational levels of $^2\Sigma$ ground-state molecules. The technique is applicable to both odd neutron and odd proton nuclei over a wide range of mass numbers A, residing in experimentally convenient diatomic systems. We estimate a 10% measurement of the NSD-PNC effect in ^{137}BaF, our first candidate, in less than 10 min of integration time. Ultimately, the techniques described here should yield values for over ten nuclear anapole moments, as well as an extraction of the previously unmeasured vector electron-axial vector neutron coupling parameter, C_{2N}, with a precision of $\sim 30\%$. The measurements will directly complement ongoing experiments studying PNC in electron-nucleon scattering.

I. INTRODUCTION

The effects of nuclear spin-dependent parity nonconservation (NSD-PNC) are of relevance in both nuclear and particle physics. These observable effects arise primarily from two underlying physical causes: *fundamental couplings of the Z^0 boson* (parameterized by the constants $C_{2P,N}$, and *nuclear anapole moments.*[1, 2] A nuclear anapole moment is a P-odd electromagnetic moment that appears due to weak interactions between nucleons. Besides being of intrinsic interest, anapole moments can provide a new method for experimentally investigating purely hadronic weak interactions.[3, 4] Only a single measurement of a nuclear anapole moment, that of ^{133}Cs,[5] has been made. The $C_{2P,N}$ constants, which describe the axial hadronic-vector electronic coupling of the Z^0 to protons and neutrons, are two of the most poorly characterized parameters of the Standard Model. Neither has been measured directly, and uncertainties on the measurements of linear combinations of the closely related electron-quark couplings $C_{2u,d}$ are at the level of 250% and 100%, respectively.[6, 7] In addition, it has been predicted that certain 4-Fermion contact interactions at an energy scale of ~ 12 TeV could lead to a 30% deviation in these constants from their expected values.[8] Thus, precise measurement of the $C_{2P,N}$ parameters could also provide evidence for new physics at high energy scales.

Here we outline an experimental program that will allow dramatic improvement on previous efforts to measure both nuclear anapole moments and the C_2 parameters. By exploiting the properties of diatomic molecules,[9, 10] we propose to measure the anapole moments of at least nine different nuclei. This will effectively double the number of input data points for interpreting hadronic weak interactions.[3] Furthermore, our ultimate precision in measuring the Z^0-hadron coupling constants should reach an unprecedented precision, approaching 30% on C_{2N} (as well as yielding a competitive measurement of C_{2P}).

Up to now, atomic PNC experiments have primarily focused on the nuclear-spin-*independent* PNC effect,[5, 11–28] arising from the weak charge of the nucleus ($Q_{\rm W}$) which parameterizes the axial electron-vector nucleon (A_eV_n) electroweak current-current coupling. The nucleons contribute coherently to this interaction, and $Q_{\rm W} \approx -N$, the number of neutrons. These previous atomic PNC experiments were forced to consider small changes between different hyperfine components of a spectral line in order to extract the NSD part of the PNC effect. Here, in contrast, the entire observable PNC effect is due to NSD-PNC.[29–31]

The NSD-PNC interactions are dominated by two physical mechanisms shown in Figure 1: Z_0 exchange between the electron and nucleus due to the vector electron axial-vector nucleon coupling and electromagnetic interaction between the electron and a parity-odd electromagnetic moment of the nucleus (anapole moment). We discuss each of these contributions separately.

A. Nuclear anapole moment contribution

A *nuclear* anapole moment arises from PNC electroweak interactions *within the nucleus*; the resulting perturbation to the nuclear structure creates a toroidal electromagnetic current around the axis of the nuclear spin.[2] It was pointed out in 1980 that the effect of such nuclear anapole moments could be observable in

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atomic PNC measurements, through a modification of PNC dependent on hyperfine structure (and thus on nuclear spin).[33] This suggestion was finally realized in the landmark 1997 experiment measuring PNC in ^{133}Cs, which provided the first[34] clear evidence for a NSD-PNC effect.[5, 35]

These measurements have been used to extract parameters describing the strength of purely hadronic weak interactions. The relationship between anapole moments and hadronic PNC parameters is discussed in Refs.[3, 36–40]. The PV NN interaction is typically parameterized using the meson-exchange picture of Desplanques, Donoghue, and Holstein (DDH)[41] which describes all possible hadronic PNC effects in terms of seven parameters. Figure 2 shows the relationship of anapole moment measurements to other types of hadronic PNC data. We will start with ^{137}Ba, an odd-neutron nucleus, with sensitivity to a unique linear combination of the DDH parameters. This will provide an important complement to other ongoing experiments which aim to provide new data on hadronic PNC couplings, using few-body nuclear systems: neutron spin rotation in transmission through liquid helium at NIST,[53, 54] and photon angular asymmetry in the reaction $n+p \rightarrow d+\gamma$,[55–57] and other experiments to measure nuclear anapole moments.[23, 26, 58] Consistency between these new measurements will finally provide a strict test of the theory of hadronic PNC.

B. Tree-level Z^0 exchange

The interaction in the second diagram of Figure 1, arises from the vector electron-axial vector nucleon ($V_e A_n$) current-current coupling due to Z^0 exchange. This diagram can be parameterized in terms of the two constants $C_{2u,d}$ describing the $V_e A_n$ interactions with up and down quarks, respectively. Our technique operates in the regime of very low q^2, where it is more natural to parameterize the $V_e A_n$ interactions in terms of proton and neutron couplings $C_{2P,N}$.[59, 60] Because these constants involve an axial hadronic current, substantial strong-interaction corrections are needed to connect the SM quark couplings to the physical hadron couplings. We assume that these corrections can be understood at the 30% level, consistent with the discussions in Refs.[[59–61]].

$$C_{2P} = 0.935 C_{2u} - 0.360 C_{2d} \tag{1}$$

$$C_{2N} = -0.440 C_{2u} + 0.765 C_{2d} \tag{2}$$

Measurements of the C_2 parameters are of interest for two reasons. First, these are now perhaps the least well-determined part of the Standard Model. There are only two significant experimental constraints on these quantities. The first is from the 1979 SLAC experiment on deep-inelastic electron-deuteron ($e-D$) scattering,[7] which measured the linear combination $2C_{2u} - C_{2d}$ with an uncertainty $\approx 250\%$ of the predicted value in the Standard Model[62]. The second is from the recent SAMPLE experiment[6] which used $e-D$ and $e-p$ quasi-elastic scattering to determine the quantity $C_{2u} - C_{2d}$ with an uncertainty $\approx$ 100% of its SM value[63, 64]. (Early claims of a deviation from the predicted value – which were atrributed to an unexpectedly large anapole moment of the proton – have been retracted based on a new analysis[65].) The large errors on the C_2 parameters contrast with other measurements of the electroweak parameters, nearly all of which are known at the level of $0.1-5\%$.[62]

In addition, deviations of the C_2's from their predicted values could possibly provide evidence for new physics at high energy scales. Because the C_2's are suppressed in the SM by $1 - 4\sin^2\theta_{\rm W} \approx 0.08$, even relatively imprecise measurements of their values can probe for new physics at an interesting scale. For example, it has been argued that a 30% deviation of the quantity $C_{2+} \equiv C_{2u} + C_{2d} \approx C_{2P} + C_{2N}$ from its predicted value could arise from a particular type of four-Fermi contact interaction,[8] at an energy scale $\sim$12 TeV . (*n.b.* Measurements of the C_2 parameters cannot yield a competitive determination of $\sin^2\theta_{\rm W}$ at low q^2.)

Measurements of C_{2N} (and, at lower precision, C_{2P}) are quite complementary to all other efforts in the field (see figure 3). A measurement of $C_{2N} \approx -0.43 C_{2u} + 0.76 C_{2d}$ would determine[59] a region of C_{2u}/C_{2d} parameter space different from any other experiment. We argue below that a determination with $\sim 30\%$ uncertainty seems possible. Such a result would mesh nicely with results from the ongoing experiment G0,[66] (which should improve on the error bounds of SAMPLE for $C_{2u} - C_{2d}$) and with the planned DIS-PV experiment, which will remeasure $2C_{2u} - C_{2d}$ with higher precision.

C. NSD-PNC effects in atoms and molecules

The physics of NSD-PNC effects in atomic and molecular systems can be described in terms of an effective term in the Hamiltonian felt by the valence electron(s) in the system,[2]

$$H_{\rm P} = \frac{G_{\rm F}}{\sqrt{2}} \kappa' \frac{\overrightarrow{\alpha} \cdot \mathbf{I}}{I} \delta^3(\mathbf{r}). \tag{3}$$

Here $G_{\rm F}$ is the Fermi constant, $\overrightarrow{\alpha}$ is the standard vector of Dirac matrices, $\mathbf{I}$ is the nuclear spin, and the delta function reflects the short-range nature of the interaction. We decompose the parameter κ', which describes the strength of the interaction, into three terms, each corresponding to one of the Feynman diagrams in Figure 3:

$$\kappa' = \kappa'_2 + \kappa'_Q + \kappa'_a \tag{4}$$

The first term, κ'_2, arises from the $V_e A_n$ term in the tree-level Z^0-exchange diagram. The second, κ'_Q, arises

from the coherent, combined effect of $Q_{\rm W}$ and the ordinary magnetic hyperfine interaction.[67–70] It is small and well-understood, so we will ignore it. The third, κ_a, is associated with the electromagnetic interaction with the nuclear anapole moment. In any measurement on a given nucleus, the effects of all three terms are indistinguishable; in fact, the anapole and weak charge/hyperfine effects can be considered radiative corrections to the tree-level Z^0 exchange process. (The anapole moment is peculiar and interesting in part because it is a rare case in which a radiative correction can be much larger than the tree-level process!)

Since the effects scale differently with nuclear mass number, A, it is possible to distinguish between the anapole and Z^0 exchange effects by measurements over a range of nuclei. This was originally proposed in Ref.[[71]]. In particular, κ_a and $\kappa_Q \propto A^{2/3}$, while κ_2 is independent of A. Thus, in heavy nuclei, the anapole moment dominates the NSD-PNC effect, while in light nuclei, the tree-level Z^0 exchange is the primary effect. Measurements in several heavy nuclei should be sufficient to determine the parameters of hadronic parity violation responsible for the anapole moment, to moderate accuracy; it appears $\sim 30\%$ is reasonable, based on detailed calculations of the nuclear structure needed to calculate the anapole.[4, 38, 39, 72–74] The residual effect of the anapole moment term κ_a' in light nuclei could then be subtracted away with $\sim 30\%$ uncertainty, allowing a determination of κ_2'.

These statements can be written in a compact, quantitative form using a simple shell-model description of the nucleus. For this purpose, we describe the nucleus (with angular momentum I) as a single valence nucleon (with index $\nu = N$ or P for a valence neutron or proton, respectively), with orbital angular momentum l around a spherical core of constant density. In this approximation,[40]

$$\kappa_a' = \frac{K}{I+1} \cdot \frac{9}{10} g_\nu \mu_\nu \frac{\alpha}{m_{\rm p} r_0} A^{2/3} \tag{5}$$

and

$$\kappa_2' = \frac{1/2 - K}{I+1} \cdot C_{2\nu}. \tag{6}$$

$$\tag{7}$$

Here,

$$K = (I + 1/2)(-1)^{I+1/2-l}; \tag{8}$$

$\hbar = c = 1$; $\mu_\nu(\mu_{\rm nuc})$ is the magnetic moment of the valence nucleon (entire nucleus), in nuclear magnetons; α is the fine structure constant; $m_{\rm p}$ is the proton mass; $r_0 = 1.2$ fm is the scale parameter for nuclear radius in the liquid-drop model; and $Q_{\rm W} = -N + (1 - 4\sin^2\theta_{\rm W})Z$, where N is the neutron number, Z is the proton number, and $\theta_{\rm W}$ is the weak mixing angle $\left[\sin^2\theta_{\rm W} \approx 0.23\right]$. In the Standard Model, the C_2 parameters (at tree level) are given by

$$C_{2\rm P} \approx -C_{2\rm N} \approx \lambda \left(1 - 4\sin^2\theta_{\rm W}\right)/2 \approx 0.05 \tag{9}$$

where $\lambda = g_A/g_V \approx 1.25$ is the charged-current axial coupling parameter.[75–78] (Expressions for $C_{2\rm P,N}$ including radiative corrections are given in Appendix C). Finally, g_ν is a parameter describing the strength of the hadronic PNC interaction between the valence nucleon and the nuclear core, which can be related to the fundamental parameters describing hadronic PNC discussed earlier. As discussed in Ref.[[40]], the proton-nucleus and neutron-nucleus constants may be written in terms of the DDH constants:

$$g_{\rm P} = 8.0 \times 10^4 \left[70\tilde{f}_\pi - 19.5\tilde{h}^0 + \tilde{g}_{\rm P}\right] \tag{10}$$

$$g_{\rm N} = 8.0 \times 10^4 \left[-47\tilde{f}_\pi - 18.9\,\tilde{h}^0 + \tilde{g}_{\rm N}\right] \tag{11}$$

where $\tilde{f}_\pi \equiv f_\pi - 0.12h^1_\rho - 0.18h^1_\omega$ and $\tilde{h}^0 \equiv h^0_\rho + 0.7h^0_\omega$ and $\tilde{g}_{\rm P,N}$ are small corrections.[3] We project our results will add bands both parallel to and nearly perpendicular to the existing Cs data, for the odd proton and odd neutron species, respectively, in Figure 2. At present, it is roughly expected that $g_{\rm P} \approx 4 - 6$ and $g_{\rm N} \approx -(0.2 - 1.0)$. With these numerical values, we can estimate the relative sizes of the Z^0 and anapole terms for nuclei that are accessible with our technique. This is shown for some representative cases in Table I, with $g_{\rm P} = 4.0$, $g_{\rm N} = -1.0$, and $|C_2| = 0.050$.[79] The data in this table makes it straightforward to estimate the projected uncertainties in the determination of the C_2 parameters from our experimental program. Measurements in a few heavier odd-neutron nuclei where κ is dominated by the anapole moment (such as ^{199}Hg and ^{137}Ba) should enable determination of $g_{\rm N}$ with $\sim 30\%$ uncertainty. Subsequent measurement of κ in the lightest available odd-neutron nucleus (for now, projected to be ^{87}Sr) would lead to a determination of $C_{2\rm N}$ with an uncertainty dominated by the imperfect subtraction of the anapole contribution: $\delta\, C_{2\rm N}({\rm anapole}) \approx |\kappa_a/\kappa_2| \cdot \delta\, g_{\rm N} \approx 25\%$. A similar program with odd-proton nuclei would yield $\delta\, C_{2\rm P}({\rm anapole}) \approx 60\%$. Expected uncertainties due to experimental error ($\sim 10\%$) and molecular wavefunctions ($10 - 20\%$; see below) increase these overall uncertainties only slightly. In summary, we have outlined a program for measurement of NSD-PNC effects over a broad range of nuclei. This program will result in the extraction of the C_2 parameters (particularly $C_{2\rm N}$) with unprecedented accuracy, as well as an improved understanding of the physics of nuclear anapole moments and hadronic PNC. With the motivation for these measurements in hand, we now turn to a discussion of the new experimental technique which should enable them.

II. THE TECHNIQUE

The basic idea of our technique is to study NSD-PNC in molecular transitions using laser and radiofrequency

spectroscopy. In particular, we will measure the NSD-PNC mixing between hyperfine/rotational levels of the ground electronic state, in molecules with a single valence electron in a $^2\Sigma$ state. These measurements are closely related to earlier atomic PNC experiments. However, our technique incorporates several key new features that allow dramatically enhanced sensitivity to NSD-PNC effects. In particular,

- NSD-PNC effects mix hyperfine/rotational levels of opposite parity in molecules, rather than electronic levels as in atoms (see review [31]). The energy spacing between the mixed levels is thus $\sim 10^4$ times smaller in molecules than in atoms. As is easily seen from ordinary perturbation theory in quantum mechanics, the smaller energy splitting (which appears in the denominator of the perturbing amplitude) leads to a larger PNC-induced mixing.

- The levels in $^2\Sigma$ molecules are so close that they can be further tuned - to nearly exact degeneracy – by exploiting the Zeeman effect to shift energy levels in a magnetic field.[30] Particular molecules have been chosen so that the rotational splitting $\approx 10\,\mathrm{GHz}$ is small enough for the required magnetic field to be modest, only ~ 0.5T. In such a field, the effective splitting between the levels will be determined by field inhomogeneity and/or time of flight through the apparatus. With reasonable technical controls, this tuning can reduce the effective splitting to $\sim 1\,\mathrm{kHz}$, leading to an enhancement in mixing of $\sim 10^7$ relative to the zero-field case. The overall gain in mixing by using molecules rather than atoms is ~ 11 orders of magnitude.

- Previous experiments using atomic Dy have shown[24] that it is possible to sensitively measure parity-violating effects in such nearly-degenerate levels.

- The previous work with Dy showed that it is possible to measure the PNC matrix element, H_{W}, with an accuracy $\delta H_{\mathrm{W}} \sim \Gamma\sqrt{1/N}$, where Γ is the effective frequency width of the transition and N is the total number of detectable molecules in the experiment. As discussed below, we anticipate achieving $\Gamma \approx 1\,\mathrm{kHz}$, corresponding to an interaction region $\sim 5\,\mathrm{cm}$ long, with $\sim 0.1\,\mathrm{ppm}$ magnetic field homogeneity. Recent work elsewhereciteTarbutt has quantified the flux of molecules available using a standard technique for molecular beam production.[81] Based on this work, we assume it is possible to achieve detection rates $\mathrm{d}N/\mathrm{d}t > 10^4/\mathrm{s}$ for individual rotational/Zeeman sublevels in a beam of the desired sort of free radical molecules (in a $^2\Sigma$ ground state). This leads to an anticipated sensitivity of $\delta H_{\mathrm{W}} \sim 10\,\mathrm{Hz}/\sqrt{T}$, where T is the total integration time (in seconds). Table II shows calculated values of H_{W} for a variety of molecules over a range of values of the nuclear charge Z. Remarkably, for the heaviest molecules, the NSD-PNC effect could be measured to 10% accuracy in only $\sim$2s of integration time.

III. INTERPRETATION OF NSD-PNC MOLECULAR SIGNALS

Interpretation of the NSD-PNC signals requires knowledge of the wavefunction of the valence electron in the molecule under study. We confine ourselves to molecules with a particular simple structure: a single valence electron in a $^2\Sigma$ ground state with strong $s-p$ hybridized orbitals. (These are the molecular equivalent of the alkali atoms such as Cs.) It has been argued for many years that straighforward, semi-empirical calculations of PNC effects in such simple molecules—which use molecular spectroscopic data as input—should be accurate at the level of $10-20\%$.[29, 31] The validity of this claim has been substantially confirmed in calculations of YbF.[82, 83] Intense effort has been put into YbF because of its potential application in experiments to measure the electron electric dipole moment (EDM).[84] These calculations (PNC and EDM) are closely related. One semi-empirical and three independent *ab initio* calculations have been done to calculate the effect of an electron EDM in YbF.[85–88] All four calculations agree at the 20% level. It thus seems essentially certain that the semi-empirical method for calculating electron wavefunctions in YbF is indeed valid at the claimed level of accuracy, and there is no reason to doubt that a similar accuracy is achieved for all other species of interest. *Ab initio* calculations of NSD-PNC effects have already been done in two of our candidate molecules: BaF and YbF.[89] In both cases, the *ab initio* results agree with the semi-empirical calculations at the 20% level. (In fact, since YbF is a particularly complicated case for the *ab initio* calculations (due to 4f-shell excitations);[86] it may be possible to perform calculations of higher accuracy in some of the lighter species we anticipate measuring.)

Finally, we note that in the near future there may be opportunities to calibrate directly the accuracy of the molecular calculations, by comparison of NSD-PNC effects observed in molecules and in atoms. Two of the nuclei accessible to our techniques are also the subject of ongoing *atomic* PNC measurements:[26–28] ^{137}Ba and[22, 23] ^{171}Yb, both of which should have sufficient sensitivity to observe the NSD-PNC effect. The atomic calculations for Ba are very accurate ($\sim 1\%$) and for Yb may reach $\sim 10\%$ accuracy. Comparison of the atomic and molecular results will thus provide a powerful cross-check of the calculations required for accurate extraction of the desired NSD-PNC effects.

We have identified a preliminary list of molecular species accessible to our proposed technique. The criteria we applied are as follows;

1. Simple electronic structure, with a single valence

electron in a $^2\Sigma$ state, making the molecular wavefunction calculable.

2. All necessary spectroscopic data for experimental parameter selection and wavefunction calculation are known.

3. The required magnetic field for crossing is $B < 0.6\,\mathrm{T}$, and the required electric field is in a reasonable range $0.3\,\mathrm{V/cm} < E_1 < 30\,\mathrm{V/cm}$.

4. Calculated NSD-PNC effects are large enough to enable a measurement with 10% statistical precision with integration time $T < 8\,\mathrm{hr}$. This is based on the semi-empirical calculations and the anticipated beam flux[80].

5. Isotopic abundance of desired odd isotope $> 5\%$.

In order to evaluate these criteria, it is necessary to calculate the hyperfine-rotational level structure in the presence of a strong external magnetic field, as well as the NSD-PNC effect. For these purposes, we follow exactly the techniques outlined in Ref.[[30]] (note that the basic idea for enhancing the NSD-PNC effect via Zeeman tuning was given in Refs.[[2, 30, 90]], although the experimental method proposed here is different than that discussed in these earlier works.) In particular, the relevant molecular structure is described by the effective Hamiltonian:[30–32]

$$\begin{aligned} H^0_{\mathrm{SR}} + H^{\mathrm{P}}_{\mathrm{SR}} &= B\mathbf{J}^2 + \Delta\mathbf{S}'\cdot\mathbf{J} + \mathbf{I}_1\cdot\mathbf{A}_1\cdot\mathbf{S}' \\ &+ \mathbf{I}_2\cdot\mathbf{A}_2\cdot\mathbf{S}' - 3\frac{q_0 Q_1}{8I_1(2I_1-1)}\mathbf{n}\cdot\mathbf{T}_1\cdot\mathbf{n} \\ &- D\mathbf{n}\cdot\mathbf{E} + \mu_0\mathbf{S}'\cdot\mathbf{G}\cdot\mathbf{B} \\ &+ W_2^{\mathrm{P}} g_2^{\mathrm{P}}\mathbf{n}\times\mathbf{S}'\cdot\mathbf{I}_1 W_2^{\mathrm{P}} g_2^{\mathrm{P}} \end{aligned} \tag{12}$$

For the $^2\Sigma$ molecules of interest, Hund's case b($\Lambda = 0$) holds[103] and we use

$$J = N + S \qquad \Delta = -2B + \gamma \tag{13}$$

where γ is the spin-doubling constant,[99] N is the rotational quantum number of the molecule, B is the rotational constant, I_1, I_2 are the spins of the two nuclei, A_1, A_2 are the axial hyperfine tensors,[100], the term containing Q_1 is the electric quadrupole contribution of the first (Ba) nucleus[101],$\mathbf{E},\mathbf{B}$ are the external electric and magnetic fields, $\mathbf{n}$ is the unit vector along the molecular axis, $\mathbf{S}'$ is the projection of the spin along the internuclear axis, $\mathbf{G}$ is the g-tensor. Calculation of the matrix elements of this Hamiltonian is simplified by recognizing that the PNC term and the hyperfine terms have identical structure:

$$H_{\mathrm{P}} = W_2^{\mathrm{P}} g_2^{\mathrm{P}}\mathbf{n}\times\mathbf{S}'\cdot\mathbf{I}_1 \equiv W_2^{\mathrm{P}} g_2^{\mathrm{P}}\mathbf{v}\cdot\mathbf{I}_1; \quad \mathbf{v} = \mathbf{n}\times\mathbf{S}' \tag{14}$$

$$H_{hf} = A\mathbf{S}'\cdot\mathbf{I}_1 \tag{15}$$

The molecular spin-rotational wavefunction may be described by

$$|J\Omega, F_1, F_2, M_2\rangle \tag{16}$$

$$J = S + N \tag{17}$$

$$F_1 = J + I_1 \tag{18}$$

$$F_2 = F_1 + I_2 \tag{19}$$

$$\tag{20}$$

where S is the spin of the last unpaired Ba electron, N is the rotation of the nuclei, I_1 and I_2 are the nuclear spins of the Ba and F, respectively. Ω is the projection of J_e on the internuclear axis, and M_2 is the projection of the total angular momentum F_2 in the laboratory frame. The parity quantum number has not been included yet. A parity wavefunction would be given by

$$|p\rangle = \frac{1}{\sqrt{2}}\left(|\Omega\rangle + \chi_J p\,|-\Omega\rangle\right) \tag{21}$$

where

$$\chi_J = (-1)^{J+1/2} \tag{22}$$

Calculations of the effective Hamiltonian which resulted in the data in Table III are outlined in Appendix A.

IV. PROPOSED MEASUREMENT STRATEGY

A schematic of the proposed experimental method is shown in Figure 4. The basic method follows that developed for experiments in nearly degenerate levels of atomic Dy.[24]At step (1), a beam of $^2\Sigma$ free radicals are produced by standard methods. The molecular beam pulse next crosses a state-preparation laser. This laser is tuned to resonance with an electric dipole-allowed transition of the molecule, which depletes one of the ground state sublevels via optical pumping. The beam then enters the bore of a large, solenoidal magnet. The depleted state (A) and a still-occupied ground state level (B) of opposite parity are brought to near crossing at the center of the magnet by careful tuning of the magnetic field $\mathbf{B} = B\hat{z}$. At this point the state-selected molecules traverse a region of oscillating electric field parallel to the magnetic field. Here, the field will be a static, spatially varying field, which in the moving frame of the molecules will create an oscillating electric field at a frequency $\omega \sim 25\,\mathrm{kHz}$. The electric field mixes levels A and B, inducing transitions from the initially populated level B to the depleted level A, with probability proportional to E_1^2. Interference between the electromagnetic and weak (PNC) mixing of the levels gives rise to a term proportional to E_1 in the repopulation of level A. After the molecules exit the magnet, they cross another laser

field (identical to the depletion laser) which excites the molecules that have repopulated the B state. As shown in Appendix B, the resulting fluorescence signal takes the form:

$$S(t) = c_A c_A^* = 4\sin^2\left(\frac{\Delta t}{2}\right)\left[\left(\frac{dE_1}{\omega}\right)^2 + 2\frac{H_{\rm W}}{\Delta}\frac{dE_1}{\omega}\right] \tag{23}$$

where d is the electric-dipole matrix element connecting states A and B; $H_{\rm W}$ is the PNC matrix element connecting the states; Δ is the detuning of the levels from exact degeneracy in the B-field; and t is the amount of time the molecules interact with the electric field. This is like the result in Dy, but here $t \to L/v$ and $\Gamma \to 0$ The PNC-induced asymmetry (i.e., the second term in $S(t)$) is proportional to $H_{\rm W}$; it changes sign both with the detuning Δ, and with the overall direction of the magnetic field B. The observable PNC effect is hence correlated with the rotational invariant $(\partial\mathbf{E}/\partial t)\cdot(\mathbf{B}-\mathbf{B}_c)$ where $\mathbf{B}_c$ is the magnetic field required for the levels to exactly cross in energy.

A pulse of gas is produced by a pulsed valve. The expansion of the gas pulse from the region of high pressure to vacuum leads to a cooling to temperatures as low as $\sim$ 3K. Molecules entrained in this gas pulse have been found to be cooled in their rotational degree of freedom,[91] leading to large fractional populations in the lowest hyperfine/rotational states of interest here. The free radicals will be produced and entrained in this jet by one of two methods. The simplest method, when available, is direct production of the free radical species from a stable, solid precursor (e.g. YbF from Yb/YbF_2) by laser ablation. We have produced such a beam of BaF starting with a rotating BaF_2 window positioned in front of and below the gas nozzle. Laser ablation with a pulsed YAG laser furnished the BaF radicals that were entrained in the gas pulses. When no precursor is available, the radicals can be formed by chemical reaction between a small admixture of reactive gas (e.g., SF_6) that is added to the noble gas carrier, and a pulse of metal atoms (e.g. Yb or Ba) created by ablation from a solid metal target. Both methods produced similar[80] beam fluxes of YbF (one of our target species). We have found that ablating a Ba rod yielded a similar flux of BaF in a low rotational level. A wide variety of other, more exotic species of diatomic free radicals have been produced with the same techniques[81].

V. TYPICAL PARAMETERS AND SIGNAL SIZES

To convey a quantitative sense of the anticipated typical operating conditions and signal sizes, we focus here first on a specific molecular species, BaF. BaF is experimentally convenient in many ways: it is easy to produce; tunable diode lasers are available for the optical pumping and detection; and it exhibits a relatively large NSD-PNC effect. Figure 6 shows a plot of the energy-level structure of ^{137}Ba as a function of magnetic field strength B. The $B = 0$ energy splittings and magnetic G-factors are known from previous spectroscopic studies[94, 95]. As seen in Figure 6, several crossings of opposite-parity levels occur in the range $B = 3000 - 5000$ G. For a single measurement, the field must be tuned near one such crossing. Signals from the molecules themselves, under application of a DC electric field[24] can be used to accurately locate the exact crossing points.

The electric field $\mathbf{E}(z)$ (which becomes $E(t)$ due to the motion of the molecules) will be generated by applying voltages to a stack of ring-shaped electrodes. With typical values of the electric dipole matrix element $\langle d\rangle$, this gives $dE_1 \approx 2.5$ kHz (see Table II). With these parameters, the average rate of detected photons S will be $S = F(dE_1/\omega)^2 \sim F/100$, where F would be the rate of detected photons for the full molecular beam (i.e., without laser depopulation or oscillating E-field). As mentioned before, ^{174}YbF was produced and detected, in a single hyperfine/rotational level, at a rate $F \sim 1000$/beam pulse.[80] We expect our total beam flux to be at least as large; however, our useful signals will likely be smaller, because we must use an odd isotope of relatively low abundance (11.2% for ^{137}Ba vs. 32% for ^{174}Yb) and use only the part of the beam from one Zeeman component (diminishing the signal by a factor of 4, corresponding to the multiplicity of sublevels for $I = 3/2$). Thus, we expect a full detectable count rate of $F \sim 100$/beam pulse. Our molecular beam jet will produce pulses that will expand to $\sim 300\mu$s wide at detection. The signal rate in the acceptance window is thus ~ 3 kHz, so we expect backgrounds due to dark counts to be negligible. The time-averaged signal rate S will thus be $\sim$100 photon counts/sec, which will allow us to measure the asymmetry, $\mathcal{A} = 2\xi$, which is twice the ratio of the $H_{\rm W}$-dependent term to the independent term in Equation 23 with an uncertainty $\delta\xi \sim 1/\sqrt{S} \sim 10\%/\sqrt{T}$, where T is the total integration time in seconds.

Using the semi-empirical model of molecular wavefunctions and the shell-model nuclear parameters described above, we can calculate the expected value of the weak mixing matrix element $H_{\rm W} = \langle b|H_{\rm P}|a\rangle$. A typical value for ^{137}Ba is $H_{\rm W} \approx 4$ Hz. Although we will control the detuning of the opposite parity levels, there will be a spread in detunings for the molecules contributing to our signal. A simple model for the distribution of magnetic field yields the following (see Appendix)dependence on Δ:

$$\mathcal{A} = 2\frac{H_{\rm W}}{\Gamma}\frac{\omega}{dE_1}\frac{1.2\Delta/\sqrt{2}}{1+\Delta^2/(2\Gamma^2)} \tag{24}$$

Assuming the magnetic field homogeneity can be controlled to less than $2\pi * 2000 s^{-1}$, $\omega = 2\pi v/L \approx 2\pi * 10^4 s^{-1}$, $E_1 \approx 0.4$V/cm so $dE_1/\omega \sim 0.1$, we have a maximum asymmetry of

$$\mathcal{A} \approx 3\% \tag{25}$$

The asymmetry can be measured to the target uncertainty level $\delta\mathcal{A}/\mathcal{A} < 10\%$, with integration time $T < 3\,\mathrm{min}$ for BaF. The asymmetry will be measured as a function of Δ by tuning the magnitude of B over a small range (a few mG); a true NSD-PNC asymmetry will have the dispersive shape shown in Figure 5. Occasionally, the entire magnetic field direction will be reversed in order to change the sign of the $\mathcal{A}$, and to check for systematic effects.

Most of the experimental details outlined above will be very similar for other molecular species of interest. The geometry of the beam and interaction regions will be identical. The electric dipole matrix elements d are similar for all species, as are the hyperfine/rotational splittings (dominated by rotational structure) and magnetic g-factors (dominated by electron spin); this means that the required electric and magnetic fields are similar. With foreseeable improvements in our technique (especially the development of higher-flux and/or slower molecular beam sources,[104–106] it is conceivable that it could also be extended down to lighter species.

VI. SYSTEMATIC EFFECTS

In any precision measurement of this type, systematic effects are of paramount importance. Previous experience[24] with this method suggests that systematics will be under excellent control in these experiments. The detection method employs three distinct reversals of experimental parameters (electric field $\mathbf{E}$; detuning Δ; and overall magnetic field $\mathbf{B}$), under which the PNC effect changes sign. This means that systematic effects require multiple simultaneous imperfections to survive our simplest analysis. For example, in Ref. [[24]], the only dangerous systematic effects resulted from the combined effect of a stray DC E-field and an unwanted B-field gradient that was independent of the current applied to the coils. Measurement and nulling of any such imperfections in the apparatus can be achieved by artificially enhancing one imperfection (e.g., by deliberately applying a DC E-field) to amplify the spurious effect. In Ref. [[24]], the accuracy of the nulling procedure was limited only by the statistical sensitivity of the measurement, and the systematic uncertainty was ultimately smaller than the statistical uncertainty. We expect similar results here.

We point out as well that the sensitivity to stray E-fields in these molecular systems is surprisingly small. This can be quantified by noting the size of the critical E-field needed, such that the E-field induced mixing equals the NSD-PNC induced mixing: $dE_{\mathrm{C}} = H_{\mathrm{W}}$. Control over stray fields at this level would be required if only the E-field reversal were available; however, the two other reversals typically diminish the size of the final systematic effect by a few orders of magnitude. We find typical values of $E_{\mathrm{C}} \sim 1\mathrm{mV/cm}$, and in the worst cases $E_{\mathrm{C}} \sim 0.1\mathrm{mV/cm}$.[96] Stray fields are generally easy to control at the mV/cm level, so we do not anticipate any serious difficulties..

Finally, our system provides an additional opportunity for rejection of systematics, beyond those in Ref. [[24]]. We find that the ratio d/H_{W} varies substantially in magnitude and sign, between the various crossing points accessible to each species. For example, for BaF this ratio takes the values +0.4,+0.5,-2.1, and -0.7 cm/mV, at the four accessible crossing points. These ratios are entirely a function of angular matrix elements, and depend in a trivial way on the details of molecular structure. This means that deviations from the known pattern of NSD-PNC mixings at the different crossings can be used as an additional filter for systematics.

VII. CONCLUSIONS

The program for investigation of NSD-PNC effects in a broad range of diatomic molecules has been inaugurated with BaF, and it should make it possible to measure NSD-PNC effects with unprecedented accuracy. This will provide knowledge both about intranuclear parity-violating forces, and about fundamental couplings of the Z^0 boson; measurement of the latter could be sensitive to new physics at the 10 TeV scale. These experiments build on recently-developed techniques (molecular beams, laser/rf spectroscopy, atomic parity violation, semi-empirical and various *ab initio* calculations) for related experiments. Possible systematic effects have been studied in detail in Ref. [[24]], and do not appear to be too difficult to control. Thus, we envision a new program of systematically exploring NSD-PNC effects at the low energy scales accessible to atomic and molecular physics, complementary to the research done at accelerator energies.

Optical excitation can be accomplished using the $X(v''0) \rightarrow A(v = 0)$ transition at wavelength $\lambda = 860\,\mathrm{nm}$. The transitions are sufficiently strong that $< 1\mathrm{mW}$ of laser power in each beam (depletion,detection) will be adequate.

The analytic solution to Laplace's equation with potentials distributed on the surface of a cylinder are available, resulting in the desired field, $E(z)$, with adequate homogeneity ($< 10\%$) over a cylindrical volume in the center.

APPENDIX A: CALCULATIONS

We now look for matrix elements in the form:

$$\langle J'\Omega' F_1' F_2' M_2' \left|\mathbf{v}\cdot\mathbf{I}_1\right| J\Omega F_1 F_2 M_2\rangle = \delta_{M_2' M_2}\delta_{F_2' F_2}\left\langle J'\Omega' F_1' M_1' \left|\mathbf{v}\cdot\mathbf{I}_1\right| J\Omega F_1 M_1\right\rangle \tag{A1}$$

$$= \delta_{M_2' M_2}\delta_{F_2' F_2}\delta_{M_1' M_1}\delta_{F_1' F_1}\left\langle J'\Omega' F_1 M_1 \left|\mathbf{v}\cdot\mathbf{I}_1\right| J\Omega F_1 M_1\right\rangle \tag{A2}$$

The matrix element of the scalar product of two tensor operators which operate on independent systems is given by (14.62) of [102]: so that

$$\begin{aligned}
&\langle J'\,\Omega'\,F_1\,M_1\left|\mathbf{V}\cdot\mathbf{I}\right|J\Omega\,F_1\,M_1\rangle \\
=&(-1)^{J+I+F_1}\left\{\begin{array}{ccc} J' & I & F_1 \\ I & J & 1\end{array}\right\}\langle J'\,\Omega'\left||V|\right|J\,\Omega\rangle\langle I\left||I|\right|I\rangle \\
=&(-1)^{J+I+F_1}\left\{\begin{array}{ccc} J' & I & F_1 \\ I & J & 1\end{array}\right\}\sqrt{I(I+1)(2I+1)}\langle J'\,\Omega'\left||V|\right|J\,\Omega\rangle
\end{aligned} \tag{A3}$$

using the Wigner-Eckart theorem (14.14). Using a result for axially-symmetric systems (see [97]):

$$\langle J'\,\Omega'\left||V|\right|J\,\Omega\rangle = (-1)^{J'-\Omega'}\sqrt{(2J'+1)(2J+1)}\left(\begin{array}{ccc} J' & 1 & J \\ -\Omega' & q' & \Omega\end{array}\right)\langle\Omega'\left|V_{q'}\right|\Omega\rangle \tag{A4}$$

Thus,

$$\begin{aligned}
\langle J'\,\Omega'\,F_1\,M_1\left|\mathbf{V}\cdot\mathbf{I_1}\right|J\Omega\,F_1\,M_1\rangle =&(-1)^{J+J'+I_1+F_1-\Omega'}\sqrt{I_1(I_1+1)(2I_1+1)(2J'+1)(2J+1)} \\
&\cdot\left\{\begin{array}{ccc} J' & I & F_1 \\ I_1 & J & 1\end{array}\right\}\left(\begin{array}{ccc} J' & 1 & J \\ -\Omega' & q' & \Omega\end{array}\right)\langle\Omega'\left|V_{q'}\right|\Omega\rangle
\end{aligned} \tag{A5}$$

where $\langle\Omega'\left|V_{q'}\right|\Omega\rangle$ is the matrix element in the molecular frame and does not depend on Js and Fs, and q' is the index for the spherical components $0,\pm1$. For $H_{\rm hfs}$, $V_q = s_q$ and for the $^2\Sigma_\Omega$ state $\Omega = \Sigma \rightarrow$

$$\langle\Omega'\left|S_{q'}\right|\Omega\rangle = \left\{\begin{array}{ll} \delta_{\Omega',\Omega}\cdot\Omega, & q'=0 \\ \delta_{\Omega',-\Omega}\cdot\sqrt{2}\Omega, & q'=\Omega'-\Omega=\pm1\end{array}\right.$$

For $H_{\rm P}$, $V_q' = (\mathbf{n}\times\mathbf{S})_{q'}$. Now $\mathbf{n} = (0,1,0)$ where $(q'=-1,0,1)$. So, the vector product in the spherical basis is

$$V_{q'} = \left\{\begin{array}{lcl} (\mathbf{n}\times\mathbf{S})_1 &=& in_0 S_1 \\ (\mathbf{n}\times\mathbf{S})_0 &=& 0 \\ (\mathbf{n}\times\mathbf{S})_{-1} &=& -in_0 S_{-1}\end{array}\right.$$

yielding

$$\begin{aligned}
\langle\Omega'\left|\mathbf{n}\times\mathbf{S}\right|\Omega\rangle = \left\{\begin{array}{l} 0, \Omega'=\Omega \\ iq'\langle\Omega'\left|n_0\right|\Omega'\rangle\langle\Omega'\left|S_{q'}\right|\Omega\rangle \\ \qquad\qquad = iq'\cdot1\cdot\sqrt{2}\Omega\end{array}\right.
\end{aligned} \tag{A6}$$

We proceed to calculate the effects of applied electric and magnetic fields, given by

$$H_{\rm E} = -D\mathbf{n}\times\mathbf{E} \equiv \mathbf{v}\cdot\mathbf{E}$$

$$H_{\rm B} = \mu_0\mathbf{B}\cdot(\hat{\mathbf{G}}\mathbf{S}) \equiv \mathbf{v}'\cdot\mathbf{B}$$

So, we need the matrix element of the electron vector $\mathbf{V}$:

$$\begin{aligned}
\left\langle J'\Omega'F_1{}'F_2{}'M_2{}'\left|V_q\right|J\Omega F_1F_2M_2\right\rangle &= (-1)^{F_2{}'-M_2{}'}\begin{pmatrix} F_2{}' & 1 & F_2 \\ -M_2{}' & q & M_2 \end{pmatrix} \\
&\cdot\left\langle J'\Omega'F_1{}'F_2{}'\left||V|\right|J\Omega F_1F_2\right\rangle \\
&= (-1)^{F_2{}'-M_2{}'}\begin{pmatrix} F_2{}' & 1 & F_2 \\ -M_2{}' & q & M_2 \end{pmatrix}\sqrt{(2F_2{}'+1)(2F_2+1)}\begin{Bmatrix} F_1{}' & F_2{}' & I_2 \\ F_2 & F_1 & 1 \end{Bmatrix} \\
&\cdot\left\langle J'\Omega'F_1{}'\left||V|\right|J\Omega F_1\right\rangle(-1)^{F_1{}'+I_2+F_2+1} \\
&= (-1)^{F_2{}'-M_2{}'}\begin{pmatrix} F_2{}' & 1 & F_2 \\ -M_2{}' & q & M_2 \end{pmatrix}\sqrt{(2F_2{}'+1)(2F_2+1)(2F_1{}'+1)(2F_1+1)}\begin{Bmatrix} F_1{}' & F_2{}' & I_2 \\ F_2 & F_1 & 1 \end{Bmatrix} \\
&\cdot\begin{Bmatrix} J' & F_1{}' & I_1 \\ F_1 & J & 1 \end{Bmatrix}(-1)^{F_1{}'+I_2+F_2+1}(-1)^{J'+I_1+F_1+1}\left\langle J'\Omega'\left||V|\right|J\Omega\right\rangle
\end{aligned}$$

Using equation (14.69) from [102] twice. Using the result from [97] again, we have

$$\begin{aligned}
&= (-1)^{F_2{}'+F_2+F_1{}'+F_1+I_1+I_2-M_2{}'+\Omega'}\begin{pmatrix} F_2{}' & 1 & F_2 \\ -M_2{}' & q & M_2 \end{pmatrix} \\
&\cdot\sqrt{(2F_2{}'+1)(2F_2+1)(2F_1{}'+1)(2F_1+1)(2J'+1)(2J+1)}\begin{pmatrix} J' & 1 & J \\ -\Omega' & q' & \Omega \end{pmatrix} \\
&\cdot\begin{Bmatrix} F_1{}' & F_2{}' & I_2 \\ F_2 & F_1 & 1 \end{Bmatrix}\begin{Bmatrix} J' & F_1{}' & I_1 \\ F_1 & J & 1 \end{Bmatrix}\left\langle\Omega'\left|V_{q'}\right|\Omega\right\rangle
\end{aligned} \tag{A7}$$

For $H_{\mathrm{E}},\ \mathbf{v}=\mathbf{n}=(0,1,0)$, so

$$\left\langle\Omega'\left|V_{q'}\right|\Omega\right\rangle = \begin{cases} 1, q'=0 \\ 0, q'=\pm 1 \end{cases}$$

whereas for $H_{\mathrm{B}},\ \mathbf{v}=\hat{\mathbf{G}}\cdot\mathbf{S}$, where

$$\hat{\mathbf{G}} = \begin{pmatrix} G_\perp & & \\ & G_\perp & \\ & & G_\parallel \end{pmatrix}$$

and we have

$$\left\langle\Omega'\left|V_{q'}\right|\Omega\right\rangle = \begin{cases} G_\parallel\cdot\Omega, q'=0 \\ \sqrt{2}G_\perp\cdot\Omega, q'=\pm 1 \end{cases}$$

We now consider the second hyperfine term due to the non-metal atom:

$$\begin{aligned}\left\langle J'\Omega' {F_1}' {F_2}' {M_2}' \left|\mathbf{V}\cdot\mathbf{I_2}\right| J\Omega F_1 F_2 M_2\right\rangle &= (-1)^{F_1+I_2+F_2}\left\{\begin{array}{ccc} {F_1}' & I_2 & F_2 \\ I_2 & F_1 & 1\end{array}\right\} \\ &\cdot\left\langle {F_1}'\Omega'\left|\left|V\right|\right|F_1\Omega\right\rangle\left\langle I_2\left|\left|I\right|\right|I_2\right\rangle \\ &= (-1)^{F_1+I_2+F_2}\left\{\begin{array}{ccc} {F_1}' & I_2 & F_2 \\ I_2 & F_1 & 1\end{array}\right\}(-1)^{J'+I_1+F_1+1}\left\langle J'\Omega'\left|\left|V\right|\right|J\Omega\right\rangle\sqrt{(2F_1+1)(2{F_1}')} \\ &\cdot\left\{\begin{array}{ccc} J' & {F_1}' & I_1 \\ F_1 & J & 1\end{array}\right\}\sqrt{I_2(I_2+1)(2I_2+1)} \\ &= (-1)^{2F_1+I_1+I_2+F_2+J'+1}\left\{\begin{array}{ccc} {F_1}' & I_2 & F_2 \\ I_2 & F_1 & 1\end{array}\right\}\left\{\begin{array}{ccc} J' & {F_1}' & I_1 \\ F_1 & J & 1\end{array}\right\}\sqrt{(2F_1+1)(2{F_1}')}\sqrt{I_2(I_2+1)(2I_2+1)} \\ &\cdot\left\langle J'\Omega'\left|\left|V\right|\right|J\Omega\right\rangle\sqrt{(2F_1+1)(2{F_1}')} \\ &= (-1)^{2F_1+I_1+I_2+F_2+2J'+1-\Omega'}\sqrt{(2F_1+1)(2{F_1}')(2J'+1)(2J+1)I_2(I_2+1)(2I_2+1)} \\ &\cdot\left\{\begin{array}{ccc} {F_1}' & I_2 & F_2 \\ I_2 & F_1 & 1\end{array}\right\}\left\{\begin{array}{ccc} J' & {F_1}' & I_1 \\ F_1 & J & 1\end{array}\right\}\left(\begin{array}{ccc} J' & 1 & J \\ -\Omega' & q' & \Omega\end{array}\right)\left\langle\Omega'\left|{V_q}'\right|\Omega\right\rangle\end{aligned} \tag{A8}$$

The quadrupole hyperfine term H_Q is given by

$$H_Q = -3\frac{q_0 Q_1}{8I_1(2I_1-1)}\mathbf{n}\hat{\mathbf{T}}_\mathbf{1}\mathbf{n} \tag{A9}$$

where the tensor $\hat{T}_1 = I_i^1 I_k^1 + I_k^1 I_i^1 - \frac{2}{3}\delta_{ik}I_1(I_1+1)$. We can rewrite $\mathbf{n}\hat{\mathbf{T}}_\mathbf{1}\mathbf{n}$ as

$$\begin{aligned} n_i T_{ik} n_k = T_{ik} n_i n_k &= T_{ik}\left(n_i n_k - \frac{1}{3}\delta_{ik}\right) \equiv T_{ik}P_{ik} \\ &= (-1)^q T_q^{(2)} P_{-q}^{(2)}\end{aligned} \tag{A10}$$

The matrix element of this scalar product is

$$\begin{aligned}\left\langle J'\Omega' {F_1}' {F_2}' {M_2}'\left|T^{(2)}\cdot P^{(2)}\right| J\Omega F_1 F_2 M_2\right\rangle &= \delta_{M_2' M_2}\delta_{F_2' F_2}\delta_{M_1' M_1}\delta_{F_1' F_1} \\ = \delta_{M_2' M_2}\delta_{F_2' F_2}\delta_{M_1' M_1}\delta_{F_1' F_1}(-1)^{J+I_1+F_1}&\left\{\begin{array}{ccc} J' & I_1 & F_1 \\ I_1 & J & 2\end{array}\right\}\left\langle J'\Omega'\left|\left|P^{(2)}\right|\right|J\Omega\right\rangle\left\langle I_1\left|\left|T^{(2)}\right|\right|I_1\right\rangle\end{aligned}$$

The first double-bar matrix element above may be found in the same manner [97]:

$$\left\langle J'\Omega'\left|\left|P^{(2)}\right|\right|J\Omega\right\rangle = (-1)^{J'-\Omega'}\sqrt{(2J'+1)(2J+1)}\left(\begin{array}{ccc} J' & 2 & J \\ -\Omega' & q' & \Omega\end{array}\right)\left\langle\Omega'\left|P_{q'}^{(2)}\right|\Omega\right\rangle \tag{A11}$$

In the molecular frame $\mathbf{n} = (0,0,1)$, so the cartesian tensor

$$P = n_i n_k - \frac{1}{3}\delta_{ik} = \frac{1}{3}\begin{pmatrix} -1 & & \\ & -1 & \\ & & 2\end{pmatrix}$$

It is straightforward to show that the spherical tensor term in the molecular frame is given by

$$P_0^2 = \sqrt{\frac{3}{2}}P_{zz} = \sqrt{\frac{3}{2}}\cdot\frac{2}{3} = \sqrt{\frac{2}{3}} \tag{A12}$$

So,

$$\langle \Omega' \left| P_0^2 \right| \Omega \rangle = \delta_{\Omega'\Omega} \cdot \sqrt{\frac{2}{3}} \tag{A13}$$

Writing T_{ik} in spherical tensor notation for the particular component T^2_{-2} gives

$$T^2_{-2} = 2I_{-1}I_{-1} \tag{A14}$$

The matrix element of T^2_{-2} is nonzero between

$$\begin{aligned} \langle II-2 \left| 2I_{-1}I_{-1} \right| II \rangle &= \langle II-2 \left| 2I_{-1} \right| II-1 \rangle \langle II-1 \left| I_{-1} \right| II \rangle \\ &= 2\sqrt{I(2I-1)} \end{aligned} \tag{A15}$$

The result is

$$\langle I_1 \left|\left| T^{(}2) \right|\right| I_1 \rangle = \sqrt{\frac{2}{3}} \sqrt{I_1(I_1+1)(2I_1+1)(2I_1-1)(2I_1+3)} \tag{A16}$$

Putting this all together for the quadrupole hyperfine term gives

$$\begin{aligned} &\langle J'\Omega' {F_1}' {F_2}' {M_2}' \left| H_Q \right| J\Omega F_1 F_2 M_2 \rangle \\ &= \delta_{{M_2}' M_2} \delta_{{F_2}' F_2} \delta_{{F_1}' F_1} \delta_{\Omega'\Omega} (-1)^{J+J'+I_1+F_1+\Omega'} \sqrt{(2J'+1)(2J+1)} \begin{pmatrix} J' & -\Omega' & 2 \\ 0 & J & \Omega \end{pmatrix} \\ &\cdot \begin{Bmatrix} J' & I_1 & I_1 \\ J & F_1 & 2 \end{Bmatrix} \cdot 3 \cdot \frac{2}{3} \sqrt{I_1(I_1+1)(2I_1+1)(2I_1-1)(2I_1+3)} \frac{q_0 Q}{8I_1(2I_1-1)} \end{aligned} \tag{A17}$$

APPENDIX B: CALCULATION OF SIGNAL

Following the method for calculating the Stark-PNC interference term used in the Dy work,[24] we will describe the time evolution of a two-level system consisting of levels brought close to crossing by the Zeeman effect. The Hamiltonian may be written

$$\begin{pmatrix} 0 & iH_{\mathrm{W}} + dE \\ -iH_{\mathrm{W}} + dE & \Delta \end{pmatrix} \tag{B1}$$

where Δ is the detuning from exact crossing of the unperturbed molecular states of opposite parity. Unlike the states in involved for Dy, we do not include a decay term since these molecules are prepared in electronic and vibrational ground states with effectively infinite lifetimes. We write the wavefunction as

$$\psi(t) = c_A(t) \left| A \right\rangle + e^{-i\Delta t} c_B(t) \left| B \right\rangle, \tag{B2}$$

with the Schrödinger equation yielding two first order equations:

$$\begin{aligned} \dot{c}_A &= -ic_B \left(dE + iH_{\mathrm{W}} \right) e^{-i\Delta t} \\ \dot{c}_B &= -ic_A \left(dE - iH_{\mathrm{W}} \right) e^{i\Delta t} \end{aligned} \tag{B3}$$

We initially depopulate $|A\rangle$, so $c_B(0) = 1$ and $c_A(0) = 0$. Now, assume that c_A is never large, so $\dot{c}_B$ is small, and $c_B \approx 1$ always; thus

$$\dot{c}_A = -i \left(dE + iH_{\mathrm{W}} \right) e^{-i\Delta t} \tag{B4}$$

Now let

$$\mathbf{E} = \mathbf{E_1} \sin(\omega t) \tag{B5}$$

Integrating equation B4 with the assumption $\Delta \ll \omega$, we find

$$c_A(t) = -2ie^{-\frac{i\Delta t}{2}} \cdot \left[\frac{dE_1}{\omega}\cos\left(\frac{\Delta t}{2}\right)\sin^2\left(\frac{\omega t}{2}\right) + i\sin\left(\frac{\Delta t}{2}\right)\left\{\frac{H_{\mathrm{W}}}{\Delta} + \frac{dE_1}{\omega}\cos^2\left(\frac{\omega t}{2}\right)\right\}\right] \tag{B6}$$

To maximize sensitivity to H_{W}, we choose $\omega t/2 = N\pi$ (where N is an integer) so that $\cos^2(\omega t/2) = 1$. If the interaction region is defined as L-long where we apply the electric field, and there are N periods of the spatially varying sinusoidal field, the molecules will experience a time-dependent field with $\omega = 2\pi N v/L$ for a time $t = L/v$. Note that $\omega t/2$ is a velocity-independent πN. Equation B6 becomes

$$c_A(t) = 2e^{-\frac{i\Delta t}{2}}\sin\left(\frac{\Delta t}{2}\right)\left(\frac{H_{\mathrm{W}}}{\Delta} + \frac{dE_1}{\omega}\right) \tag{B7}$$

The population transferred to $|A\rangle$ from $|B\rangle$ is

$$|c_A|^2 = 4\sin^2\left(\frac{\Delta t}{2}\right)\left[\left(\frac{H_{\mathrm{W}}}{\Delta} + \frac{dE_1}{\omega}\right)^2\right] \tag{B8}$$

Expanding and ignoring small terms $O\left[(H_{\mathrm{W}}/\Delta)^2\right]$, we have

$$|c_A|^2 = 4\sin^2\left(\frac{\Delta t}{2}\right)\left[2\frac{H_{\mathrm{W}}}{\Delta}\frac{dE_1}{\omega} + \left(\frac{dE_1}{\omega}\right)^2\right] \tag{B9}$$

The ratio ξ of the PNC-Stark interference term to the leading Stark term is

$$\xi = 2\frac{H_{\mathrm{W}}}{\Delta}\frac{\omega}{\mathrm{d}E_1} \tag{B10}$$

Equation (B10) diverges as $\Delta \to 0$, suggesting that the asymmetry can be made arbitrarily large. However, under realistic conditions this is not possible. In particular, magnetic field inhomogeneities over the volume of interest leads to an effective distribution in values of Δ, which averages ξ (which is odd in Δ) to zero for small average detunings. To show this behavior explicitly, we take a simple model where the magnetic field distribution is a Gaussian. We must sum the contributions to the signal due to molecules that experience these different fields. Including Γ as an effective width of the detuning distribution, we integrate Equation B9 against

$$f(\Delta) = \frac{e^{-[(\Delta-\Delta_0)/(\sqrt{2}\Gamma)]^2}}{\Gamma\sqrt{2\pi}} \tag{B11}$$

Using the additional simplifying assumption $\sin\Delta t/2 \approx \Delta t/2$, we find the volume averaged value of $|c_A|^2$

$$\overline{|c_A|^2} \approx \frac{dE_1}{\omega}t^2\left[2H_{\mathrm{W}}\Delta_0 + \frac{dE_1}{\omega}\left(\Delta_0^2 + \Gamma^2\right)\right] \tag{B12}$$

The ratio ξ of equation B10 now becomes

$$\overline{\xi} = 2\frac{H_{\mathrm{W}}}{\Delta_0}\frac{\omega}{\mathrm{d}E_1}\frac{\Delta_0^2}{\Delta_0^2 + \Gamma^2} \tag{B13}$$

The asymmetry $\mathcal{A} \equiv 2\xi$ is hence maximized at $\Delta_0 = \Gamma$ and is

$$\mathcal{A} = 2\frac{H_{\mathrm{W}}}{\Gamma}\frac{\omega}{dE_1} \tag{B14}$$

(see Figure 5.) Finally, we note in passing that integrating Equation (B12) against a typical supersonic beam velocity profile (longitudinal velocity $\sim$ 400m/s, velocity width $\sim$ 40m/s) introduces a negligible change in the asymmetry.

APPENDIX C: C2S

For reference purposes, here are the constants and their relations to SM parameters:

$$C_{2u} = 2g_V^e g_A^u = -\frac{1}{2} + 2\sin^2\theta_{\rm W}$$

$$C_{2d} = 2g_V^e g_A^d = \frac{1}{2} - 2\sin^2\theta_{\rm W}$$

$$C_{2p} = C_{2u} + C_{2d}$$

$$C_{2m} = C_{2u} - C_{2d}$$

$$C_{2P} = 2FC_{2u} + (F-D)C_{2d}[60]$$

$$C_{2N} = (F-D)C_{2u} + 2FC_{2d}$$

$$F \approx 0.425 \qquad D \approx 0.825 \qquad g_A = F + D \approx 1.25 \tag{C1}$$

Axial-vector-current anomaly induces axial-vector isoscalar neutral current which leads to[59]

$$\Delta C_{2u} = \Delta C_{2d} \approx 0.10\, C_{2u} \approx -0.10\, C_{2d} \rightarrow$$

$$C_{2P} = 2F\, 1.1\, C_{2u} + (F-D)\, 0.9\, C_{2d}$$

$$= 0.935 C_{2u} - 0.360 C_{2d}$$

$$C_{2N} = (F-D)1.1 C_{2u} + 2F 0.9 C_{2d}$$

$$= -0.440 C_{2u} + 0.765 C_{2d} \tag{C2}$$

Including radiative corrections

$$C_{2u} = -0.0360$$

$$C_{2d} = 0.0265 \tag{C3}$$

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TABLE I: Shell-model values of parameters for some accessible nuclei. I is the nuclear angular momentum. The valence nucleon in the shell model is ν = N,P. The orbital angular momentum of ν is l. The parameter describing the strength of coupling between the nuclear anapole moment and the electron spin is κ_a. The parameter describing the strength of the $V_e A_n$ term in Z^0 exchange is κ_2. We take $g_{\rm P} = 4$ and $g_{\rm N} = -1$ for this calculation.

Nucleus	I	ν	l	$100 \times \kappa_a$	$100 \times \kappa_2$	$\lvert\kappa_a/\kappa_2\rvert$
$^{87}Sr_{38}$	9/2	N	4	−3.9	5.0	0.8
$^{137}Ba_{56}$	3/2	N	2	−4.6	3.0	1.5
$^{173}Yb_{70}$	5/2	N	3	−4.5	3.6	1.3
$^{199}Hg_{80}$	1/2	N	1	−5.0	1.7	2.9
$^{201}Hg_{80}$	3/2	N	1	−6.0	5.0	1.2
$^{27}Al_{13}$	5/2	P	2	10.0	−5.0	2.0
$^{69}Ga_{31}$	3/2	P	1	17.0	−5.0	3.4
$^{81}Br_{35}$	3/2	P	1	19.0	−5.0	3.8
$^{115}In_{49}$	9/2	P	4	27.0	−5.0	5.2

TABLE II: A partial list of molecular species accessible to this technique (according to the criteria described in the text). "# of crossings" is the number of distinct energies at which levels of opposite parity cross, for $B < 0.6$T. "Range of B" is the variation of field strength needed to access all crossing points. (A complete set of crossings has not been calculated yet for AlS or SrF.) "$T(10\%)$" is the anticipated integration time to reach a statistical sensitivity of 10% in the NSD-PNC measurement for that species, with assumptions as described in the text.

Species	Nuclei	# of crossings	Range of B [T]	$T(10\%)$
SrF	^{87}Sr	≥ 4	$0.35 - 0.5$	< 100 min
BaF	^{135}Ba, ^{137}Ba	4	$0.32 - 0.44$	< 10 min
YbF	^{171}Yb, ^{173}Yb	2	$0.33 - 0.5$	< 1 min
HgF	^{199}Hg, ^{201}Hg	4,2	$0.13 - 0.30$	< 1 min
AlS	^{27}Al	≥ 3	$0.4 - 0.6$	< 100 min
GaO	^{69}Ga, ^{71}Ga	3	$0.46 - 0.55$	< 10 min
MgBr	^{79}Br, ^{81}Br	3	$0.34 - 0.37$	< 100 min
InO	^{115}In	5	$0.44 - 0.53$	< 1 min

TABLE III: $^2\mathbf{\Sigma}_{1/2}$ molecules with known parameters of the spin-rotational Hamiltonian (MHz)

	I_1	I_2	B	γ	$A_{1\parallel}$	$A_{1\perp}$	$A_{2\parallel}$	$A_{2\perp}$	eqQ
^{87}SrF	9/2	1/2	7515	75	−576	−556	127	97	−146
^{137}BaF	3/2	1/2	6480	81	2453	2401	67	59	−117
^{171}YbF	1/2	1/2	7246	13	7822	7513	220	134	
^{199}HgF	1/2	1/2			22621	21880			
^{201}HgF	3/2	1/2			−8054	−7760			
^{27}AlS	5/2	0	8369	66	933	764	0	0	−24
^{69}GaO	3/2	0	8217	839	1736	1356	0	0	
^{71}GaO	3/2	0	8172	839	2207	1722	0	0	
Mg^{79}Br	0	3/2	4972	178	0	0	310	103	110
Mg^{81}Br	0	3/2	4944	177	0	0	334	111	92
^{115}InO	9/2	0	9788	3831	1832	1070	0	0	−651

TABLE IV: Parity non-conserving amplitudes at the crossings of the spin-rotational levels in magnetic field

	I	κ_a	W_P (Hz)	F_z	$B_{\rm cross}$ (Gs)	$\left\lvert\frac{\langle \boldsymbol{n}\times\boldsymbol{s}\cdot\boldsymbol{I}\rangle}{I}\right\rvert$	$\lvert\langle\text{PNC}\rangle\rvert$ (Hz)	$\lvert D\langle\mathbf{n}\rangle\rvert$ $\left(\frac{\text{kHz}}{\text{V/cm}}\right)$
^{137}BaF	3/2	−0.06	164	5/2	3250	0.44	4.0	2.7
				3/2	3550	0.34	3.0	1.5
				3/2	3930	0.22	1.9	3.9
				−1/2	4330	0.39	3.5	1.5
^{171}YbF	1/2	−0.07	729	3/2	3310	0.52	17	1.7
				1/2	3370	0.52	17	0.4
^{199}HgF	1/2	−0.08	2517	3/2	2650	0.62	79	10
				3/2	2690	0.46	58	11
				1/2	2730	0.46	58	11
				1/2	2890	0.29	37	4
				−1/2	2930	0.29	37	4
^{201}HgF	3/2	−0.08	2559	1/2	1285	0.43	66	18
				3/2	1345	0.43	66	17
^{69}GaO	3/2	0.21	61	2	4950	0.43	4.4	30
				1	5290	0.34	3.6	7
				1	5430	0.19	2.0	36
^{71}GaO	3/2	0.22	61	2	4690	0.43	4.7	28
				1	5050	0.34	3.7	9
				1	5270	0.20	2.2	36
^{115}InO	9/2	0.30	181	5	4430	0.42	21	98
				4	4770	0.35	18	110
				4	4890	0.22	11	26
				3	5130	0.27	14	120
				3	5270	0.29	15	33

FIG. 1: Feynman diagrams of 2 of the processes contributing to NSD-PNC. (a) Tree-Level Z^0 exchange ($V_e A_n$ term). (b) Z^0 and $W^{\pm}$ exchange within the nucleus gives rise to the nuclear anapole moment (indicated by the blue ellipse) along the nuclear angular momentum $\mathbf{I}$, which couples magnetically to the electron spin σ_e.

FIG. 2: Current status of hadronic PNC parameters. This figure, reproduced from [3], shows the ranges of values of a particular linear combination of these parameters for the two anapole experiments on Cs and Tl, pp scattering experiments.[42–45], a pα scattering experiment [46, 47], a γ-ray circular polarization in ^{18}F experiment[48, 49], and angular asymmetry for polarized ^{19}F decay[50, 51]. The size of the plot indicates the DDH "reasonable range" for these particular linear combinations. Note the poor agreement of the ^{133}Cs and ^{205}Tl bands with the other data. The green dot corresponds to the theoretical "best values". As indicated by Holstein[52], a consistent set of couplings is not produced. Our measurements could add over a dozen new bands to this plot, similar to those shown in light pink and blue (approximately equal numbers of each type). (Figure reproduced from [3]).

FIG. 3: Current status of C_2 parameters. The orange dot represents the Standard Model prediction[63]. The blue band is from the 1979 SLAC e-D deep inelastic scattering experiment[7]. The red band is from the SAMPLE experiment at MIT Bates.[6, 64, 65]. The green and yellow bands indicate the projected sensitivity of our experiments, for measurements on protons and neutrons, respectively.

FIG. 4: Schematic of the apparatus (top) and evolution of state populations (bottom). (1): molecules are formed by laser ablation into a pulsed jet; states a and b have equal thermal populations. (2): a laser beam (green) depopulates state a by optical pumping. (3): a spatially varying E-field is applied parallel to the B-field formed by the solenoid. (4): population transferred to state a by the E-field is probed by laser-induced fluorescence.

FIG. 5: Simulated Asymmetry. The asymmetry ξ appears as the difference in peak heights of the signal divided by the average when the oscillating E-field is of different signs. The plot shows the change in ξ as a function of the decrossing Δ_0, where the asymmetry reflects the inhomogeneity of the magnetic field. The depicted maximum asymmetry $\sim 8\%$ is the actual size expected under typical conditions for the first molecular species we will study, ^{137}Ba.

FIG. 6: Hyperfine/rotational energy levels of ^{137}BaF in a magnetic field B. Red(green) lines correspond to levels of even(odd) parity arising from states with rotational quantum number $N = 0(N = 1)$. Multiple crossings occur in the range indicated by the orange ellipse; many of these are between states with the same value of m_F; (projection of the total angular momentum along $\mathbf{B}$), and thus can be mixed by H_{W}.