

Combined effect of coherent Z exchange and the hyperfine interaction in the atomic parity-nonconserving interaction

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The nuclear spin-dependent parity-nonconserving (PNC) interaction arising from a combination of the hyperfine interaction and the coherent, spin-independent, PNC interaction from Z exchange is evaluated using many-body perturbation theory. For the $6s_{1/2}$ - $7s_{1/2}$ transition in ^{133}Cs , we obtain a result that is about 40% smaller than that found previously by Bouchiat and Piketty [Phys. Lett. B **269**, 195 (1991)]. Applying this result to ^{133}Cs leads to an increase in the experimental value of nuclear anapole moment and exacerbates differences between constraints on PNC meson coupling constants obtained from the Cs anapole moment and those obtained from other nuclear parity violating experiments. Nuclear spin-dependent PNC dipole matrix elements, including contributions from the combined weak-hyperfine interaction, are also given for the $7s_{1/2}$ - $8s_{1/2}$ transition in ^{211}Fr and for transitions between ground-state hyperfine levels in K, Rb, Cs, Ba^+ , Au, Tl, Fr, and Ra^+ .

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I. INTRODUCTION

The precise measurements of the $6s[F=4]$ - $7s[F=3]$ and $6s[F=3]$ - $7s[F=4]$ parity-nonconserving (PNC) dipole matrix elements in ^{133}Cs by Wood *et al.* [1] lead to a value of the weak charge $Q_W^{\text{exp}}(^{133}\text{Cs}) = -72.73(46)$, which is in agreement with the standard model value $Q_W^{\text{SM}}(^{133}\text{Cs}) = -73.09(3)$ [2]. (The experimental value includes a net correction of -1.1% to the theoretical PNC amplitude [3–5] from the Breit interaction [6], αZ vertex corrections [7,8], Coulomb-field vacuum polarization [9], and nuclear skin effects [10,11].) These measurements also lead to an experimental value of the much smaller contribution from the nuclear spin-dependent PNC interaction that is accurate to about 15%. This spin-dependent contribution has three distinct sources: the nuclear anapole moment [12,13], the Z exchange interaction from nucleon axial-vector ($A_n V_e$) currents, and the combined action of the hyperfine interaction and the spin-independent Z exchange interaction from nucleon vector ($V_n A_e$) currents [14,15]. Of these three, the anapole contribution dominates. The contributions from the anapole and nuclear axial-vector current are

$$H^{(i)} = \frac{G}{\sqrt{2}} \kappa_i \boldsymbol{\alpha} \cdot \mathbf{I} \rho(r), \quad (1)$$

where G is the universal weak coupling constant, \mathbf{I} is the nuclear spin, and $\rho(r)$ is a normalized nuclear density function. The subscript i of the dimensionless constants κ_i takes the values $i=a$ for the anapole contribution and $i=2$ for the axial-vector contribution. In Refs. [14,15], the hyperfine-vector current contribution was also reduced to the form given in Eq. (1) with a corresponding dimensionless constant κ_{hf} .

To extract the anapole contribution κ_a from experiment, it is necessary to know the corresponding spin-dependent PNC amplitude calculated with $\kappa_a=1$, as well as the two contributions from the axial-vector and weak-hyperfine interference terms quantified by κ_2 and κ_{hf} . The spin-dependent PNC amplitude was calculated in various approximations in Refs. [3,16,17]. Nuclear shell-model values of κ_2 for ^{133}Cs and ^{203}Tl were obtained in recent calculations by Haxton *et al.* [18]. An analytical approximation for κ_{hf} was derived by Flambaum and Khriplovich [14] and values of κ_{hf} were later determined for various cases of experimental interest by Bouchiat and Piketty [15].

Recently, Haxton and Wieman [19] used the values of κ_2 and κ_{hf} determined as described above to extract values of κ_a from PNC measurements in ^{133}Cs [1]. (In Ref. [19], κ_2 and κ_{hf} are designated by κ_{Z_0} and κ_{Q_W} , respectively.) The resulting anapole moments were, in turn, used to place constraints on PNC meson coupling constants [20]. The constraints obtained from the Cs experiment were found to be inconsistent with constraints from other nuclear PNC measurements, which favor a smaller value of the ^{133}Cs anapole moment.

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Motivated by this disagreement, we are led to reexamine the combined hyperfine-weak interaction. We find that the contribution of this term to the PNC dipole matrix element at the Dirac-Hartree-Fock (DHF) level can be approximated by a spin-dependent interaction of the type given in Eq. (1); however, such an approximation is not justified in correlated calculations, since contributions from Eq. (1) are very sensitive to correlations, whereas contributions from the combined hyperfine-weak interaction are relatively insensitive to correlation corrections. We do find, nevertheless, that even in correlated calculations there is a rough proportionality between contributions from the combined interaction and those from the interaction given in Eq. (1) that is independent of hyperfine state, and we use this fact to define “effective” values of the coupling strength κ_{hf} for cases of potential experimental interest. For the $6s-7s$ transition in Cs, our effective value of κ_{hf} is about 40% smaller than the value from Ref. [15]. Interestingly, for this case our final correlated value of κ_{hf} is quite close to the value predicted by the formula derived in Ref. [14]. Other things being unchanged, this decrease in the size of κ_{hf} leads to an increase in the size of κ_a and, correspondingly, in the Cs anapole moment; consequently, increasing the inconsistencies between various experimental constraints on PNC meson coupling constants described in Ref. [19].

II. METHOD

We write the spin-dependent PNC correction to the reduced electric-dipole matrix element $\langle wF_F \| z \| vF_I \rangle$ as the sum of three terms:

$$\langle wF_F \| z \| vF_I \rangle_{\text{PNC}}^{\text{sd}} = \kappa_a \langle wF_F \| z \| vF_I \rangle^{(a)} + \kappa_2 \langle wF_F \| z \| vF_I \rangle^{(2)} + \langle wF_F \| z \| vF_I \rangle^{(\text{hf})}, \quad (2)$$

where indices (a), (2), and (hf) correspond to the anapole, axial-vector, and weak-hyperfine interference, respectively. Since the anapole and axial-vector contributions both take the form given in Eq. (1), we can introduce $\langle wF_F \| z \| vF_I \rangle^{(2,a)} \equiv \langle wF_F \| z \| vF_I \rangle^{(a)} = \langle wF_F \| z \| vF_I \rangle^{(2)}$. We then define κ_{hf} as the ratio

$$\kappa_{\text{hf}} = \frac{\langle wF_F \| z \| vF_I \rangle^{(\text{hf})}}{\langle wF_F \| z \| vF_I \rangle^{(2,a)}}. \quad (3)$$

We expect, and indeed find, that κ_{hf} depends on the initial and final hyperfine levels. For cases considered here, however, the dependence of κ_{hf} on the hyperfine levels F_I and F_F is weak and we may treat κ_{hf} as constant to some level of accuracy. We write the expression for the total spin-dependent PNC contribution to the electric-dipole matrix element $\langle wF_F \| z \| vF_I \rangle$ as

$$\langle wF_F \| z \| vF_I \rangle_{\text{PNC}}^{\text{sd}} = (\kappa_a + \kappa_2 + \kappa_{\text{hf}}) \langle wF_F \| z \| vF_I \rangle^{(2,a)} \quad (4)$$

and define

$$\kappa = \kappa_a + \kappa_2 + \kappa_{\text{hf}}. \quad (5)$$

In this work, we calculate both $\langle wF_F \| z \| vF_I \rangle^{(\text{hf})}$ and $\langle wF_F \| z \| vF_I \rangle^{(2,a)}$ and, therefore, determine the state-dependent values of κ_{hf} .

The hyperfine interaction Hamiltonian is written

$$H^{(\text{hf})} = -ec \boldsymbol{\alpha} \cdot \mathbf{A}, \quad \mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int d^3x \frac{\mathbf{M}(x) \times (\mathbf{r} - \mathbf{x})}{|\mathbf{r} - \mathbf{x}|^3}, \quad (6)$$

where $\mathbf{M}(x)$ is the magnetization density, which is related to the nuclear moment $\boldsymbol{\mu}_I$ by

$$\boldsymbol{\mu}_I = \int d^3x \mathbf{M}(x) = g_I \mathbf{I} \mu_N.$$

Here $\mu_N = |e| \hbar / 2M_p$ is the nuclear magneton.

The dominant, spin-independent, part of the weak interaction is

$$H^{(1)} = \frac{G}{2\sqrt{2}} Q_W \gamma_5 \rho(r), \quad (7)$$

where Q_W is the conserved weak charge of the nucleus, given at tree level in terms of the neutron number N , the proton number Z , and the Weinberg angle θ_W by $Q_W = Z(1 - 4\sin^2\theta_W) - N$, and $\rho(r)$ is a nucleon distribution function. In our numerical calculations of the interference term, we use radiatively corrected values of Q_W inferred from Ref. [2]. The nucleon distribution $\rho(r)$ is assumed to have the form

$$\rho(r) = \frac{\rho_0}{1 + \exp[(r - C)/a]}, \quad (8)$$

where $a = 0.523$ fm (corresponding to 90%–10% falloff thickness $t = 2.3$ fm) and where C is inferred from the nuclear charge radii listed in Ref. [21]. In the exceptional case of ^{211}Fr , we choose $C = 6.733$ fm, corresponding to the value $R_{\text{rms}} = 5.566$ fm given in Ref. [22]. We assume that the radial dependence of the magnetization distribution is identical to that of the nucleon distribution.

As shown in Appendix A, the dipole matrix element corresponding to the weak-hyperfine interference is given by the third-order perturbation theory expression

$$\begin{aligned}
\langle wIF_F M_F | z | vIF_I M_I \rangle^{(\text{hf})} = & \sum_{\substack{m \neq w \\ n \neq w}} \frac{\langle w | H^{(1)} | n \rangle \langle n | H^{(\text{hf})} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)(E_w - E_n)} + \sum_{\substack{m \neq w \\ n \neq w}} \frac{\langle w | H^{(\text{hf})} | n \rangle \langle n | H^{(1)} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)(E_w - E_n)} \\
& + \sum_{\substack{m \neq w \\ n \neq v}} \frac{\langle w | H^{(1)} | m \rangle \langle m | z | n \rangle \langle n | H^{(\text{hf})} | v \rangle}{(E_w - E_m)(E_v - E_n)} + \sum_{\substack{m \neq w \\ n \neq v}} \frac{\langle w | H^{(\text{hf})} | m \rangle \langle m | z | n \rangle \langle n | H^{(1)} | v \rangle}{(E_w - E_m)(E_v - E_n)} \\
& + \sum_{\substack{m \neq v \\ n \neq v}} \frac{\langle w | z | n \rangle \langle n | H^{(1)} | m \rangle \langle m | H^{(\text{hf})} | v \rangle}{(E_v - E_m)(E_v - E_n)} + \sum_{\substack{m \neq v \\ n \neq v}} \frac{\langle w | z | n \rangle \langle n | H^{(\text{hf})} | m \rangle \langle m | H^{(1)} | v \rangle}{(E_v - E_m)(E_v - E_n)} \\
& - \langle w | H^{(\text{hf})} | w \rangle \sum_{m \neq w} \frac{\langle w | H^{(1)} | m \rangle \langle m | z | v \rangle}{(E_w - E_m)^2} - \sum_{n \neq v} \frac{\langle w | z | n \rangle \langle n | H^{(1)} | v \rangle}{(E_v - E_n)^2} \langle v | H^{(\text{hf})} | v \rangle, \quad (9)
\end{aligned}$$

where we use designations $|w\rangle$ and $|v\rangle$ on the right-hand side for coupled hyperfine states $|wIF_F M_F\rangle$ and $|vIF_I M_I\rangle$, respectively, and where we designate the energy of state i by E_i . Note that the other matrix element $\langle wIF_F M_F | z | vIF_I M_I \rangle^{(2,a)}$ in Eq. (4) is obtained from a considerably simpler second-order perturbation theory-calculation.

In Ref. [15], terms on the second and fourth lines of Eq. (9) were ignored and partial sums on the first and third lines, such as

$$\sum_{n \neq v} \frac{H^{(1)} | n \rangle \langle n | H^{(\text{hf})}}{E_n - E_v},$$

were carried out using free-particle Green's functions and reduced to an effective interaction

$$H^{(\text{eff})} = \frac{G}{\sqrt{2}} \kappa_{\text{hf}} \boldsymbol{\alpha} \cdot \mathbf{I} \rho(r)$$

of the form given in Eq. (1). A similar reduction was made in Ref. [14]. Here, we evaluate all of the terms in Eq. (9) numerically. One important advantage of this direct numerical evaluation is that correlation corrections to $\langle wIF_F || z || vIF_I \rangle^{(\text{hf})}$ can be determined using standard many-body methods. Indeed, we find that Eq. (9) is insensitive to correlations at the random-phase approximation (RPA) level for most of the cases considered here, whereas calculations based on the contracted approximation above are very sensitive to correlation corrections. A reduction of Eqs. (4) and (9) to reduced matrix elements suitable for numerical evaluation is given in Appendix B.

III. NUMERICAL RESULTS

We evaluate the reduced dipole matrix element $\langle wF_F || z || vF_I \rangle^{(\text{hf})}$ given in Eq. (B14) and the reduced matrix element $\langle wF_F || z || vF_I \rangle^{(2,a)}$ given in Eq. (B15), and we find that their ratio is approximately independent of the angular-momentum quantum numbers F_I and F_F for transitions between hyperfine levels.

Let us consider the $6s$ - $7s$ transition in Cs. We first evalu-

ate the reduced matrix elements in Eqs. (B15) and (B14) at the DHF level of approximation. We solve the DHF equations in a finite B -spline basis using the methods described in Ref. [23] and use the resulting basis functions to evaluate matrix elements and carry out sums over intermediate states. For the case Cs, our basis set consists of 100 splines of order 15 for each angular-momentum state. The basis orbitals are constrained to a cavity of radius 45 a.u.; the cavity radius is modified in other atoms to accommodate the initial and final valence orbitals. As a check, we carried out the Cs calculations using a cavity of radius 75 a.u. to verify that the results are stable against changes in the cavity radius. Results of our DHF calculations for the transitions between the possible hyperfine levels are presented in the upper four rows of Table I. We find that the ratio κ_{hf} of the $\langle wF_F || z || vF_I \rangle^{(\text{hf})}$ to $\langle wF_F || z || vF_I \rangle^{(2,a)}$ matrix element changes from level to level by only 2% in the DHF approximation.

The DHF treatment of PNC in cesium is known to be a

TABLE I. We list values of κ_{hf} for transitions between hyperfine levels $6s[F_I]$ - $7s[F_F]$ in Cs determined in DHF and RPA approximations. The atomic number is $A=133$, the nuclear spin is $I=7/2$, the nuclear magnetic moment is $\mu_I=2.5826$, the weak charge (including radiative corrections) is $Q_W=-73.09(3)$, and the 50% falloff radius is $C=5.675$ fm for both the nuclear $\rho(r)$ and magnetization $M(r)$ distributions; the 10%–90% falloff distance is 2.3 fm. The PNC reduced dipole matrix elements $\langle wF_F || z || vF_I \rangle^{(2,a)}$ are given together with the weak-hyperfine interference correction to dipole matrix elements $\langle wF_F || z || vF_I \rangle^{(\text{hf})}$; their ratio is κ_{hf} . Numbers in square brackets represent powers of 10.

$F_F - F_I$	$\langle 7sF_F z 6sF_I \rangle^{(2,a)}$	$\langle 7sF_F z 6sF_I \rangle^{(\text{hf})}$	κ_{hf}
Dirac-Hartree-Fock			
3-3	1.908[−12]	1.193[−14]	6.251[−03]
3-4	5.481[−12]	3.480[−14]	6.349[−03]
4-3	4.746[−12]	3.020[−14]	6.364[−03]
4-4	2.173[−12]	1.358[−14]	6.251[−03]
Random-phase approximation			
3-3	2.249[−12]	1.141[−14]	5.076[−03]
3-4	7.299[−12]	3.579[−14]	4.903[−03]
4-3	6.432[−12]	3.139[−14]	4.880[−03]
4-4	2.560[−12]	1.300[−14]	5.076[−03]

rather poor approximation, giving a value for the dominant part of the PNC dipole matrix element that is 20% smaller than the final correlated value. To obtain a reliable value for the PNC matrix element, one must go beyond the DHF approximation and treat correlation corrections. The dominant correlation corrections, those associated with core shielding, are obtained in the random-phase approximation. Including RPA corrections to both weak-interaction and dipole matrix elements gives a value for the dominant PNC dipole matrix element in Cs that is within 2% of the final correlated value.

The RPA matrix elements are calculated as described in Ref. [24], with the value of ω in the RPA equations set to zero. In the last four rows of Table I, we give values of $\langle 7sF_F || z || 6sF_I \rangle^{(2,a)}$ that include RPA corrections to both dipole and weak-interaction operators, and values of $\langle 7sF_F || z || 6sF_I \rangle^{(hf)}$ that include RPA corrections to the dipole, weak-interaction, and hyperfine operators. While the RPA values of $\langle 7sF_F || z || 6sF_I \rangle^{(2,a)}$ are 15–25 % larger than the DHF values, the RPA and DHF values of $\langle 7sF_F || z || 6sF_I \rangle^{(hf)}$ differ by only 3–5 %. Thus, by contrast to PNC dipole matrix elements induced by the dominant spin-independent interaction and by the spin-dependent interactions given in Eq. (1), which are very sensitive to correlation corrections, the third-order matrix elements for the combined interaction are relatively insensitive to correlations for the 6s-7s transition in Cs. It should be emphasized that the contraction of operators introduced in Ref. [15] is a useful approximation at the independent-particle DHF level of approximation; however, when correlation corrections are included, although an approximate proportionality still obtains, the proportionality *constant* depends on correlations; this is a reflection of the fact that there is no effective Hamiltonian of form Eq. (1) for the combined interaction.

We include negative-energy contributions [25] when evaluating sums over intermediate states in Eqs. (B14) and (B15) and when calculating RPA matrix elements. We find almost no negative-energy correction to $\langle 7sF_F || z || 6sF_I \rangle^{(2,a)}$. However, the negative-energy corrections to $\langle 7sF_F || z || 6sF_I \rangle^{(hf)}$ were found to be large, 22–23 % at both the DHF and RPA levels of approximation. Since negative-energy contributions are important for accurate calculation of $\langle 7sF_F || z || 6sF_I \rangle^{(hf)}$, they are, therefore, important in the evaluation of κ_{hf} . Omission of negative-energy contributions leads to values of $\kappa_{hf}=0.0049$ in the DHF approximation, and $\kappa_{hf}=0.0038$ in the RPA approximation which are about 20% smaller than our final values listed in Table I. We note that our final correlated value fortuitously coincides with the DHF value without negative-energy contributions; the correlation correction decreases the value of κ_{hf} and the negative-energy contribution increases κ_{hf} by approximately the same amount. We stress again that these two effects contribute, in fact, to different quantities, negative energies contribute only to $\langle 7sF_F || z || 6sF_I \rangle^{(hf)}$, and correlation primarily to $\langle 7sF_F || z || 6sF_I \rangle^{(2,a)}$.

We also found that sums in the interference matrix element given in Eq. (B14) must include the entire set of basis orbitals, in contrast to the sums in Eq. (B15), where omitting high-energy orbitals from the basis has very little effect. In other words, the completeness of the basis is very important

TABLE II. We list values of κ_{hf} for transitions between hyperfine levels $8s[F_F]-7s[F_I]$ in Fr determined in RPA-type calculations. Here, the atomic number $A=211$, the nuclear spin is $I=9/2$, the nuclear magnetic moment is $\mu_I=4.00$, the weak charge (including radiative corrections) is $Q_w=-116.23$, and the 50% falloff radius is $C=6.7325$ fm for both the nuclear $\rho(r)$ and magnetization $M(r)$ distributions; the 10%–90% falloff distance is 2.3 fm. The PNC reduced dipole matrix elements $\langle wF_F || z || vF_I \rangle^{(2,a)}$ are given together with the weak-hyperfine interference correction to dipole matrix elements $\langle wF_F || z || vF_I \rangle^{(hf)}$; their ratio is κ_{hf} . Numbers in square brackets represent powers of 10.

F_F-F_I	$\langle 8sF_F z 7sF_I \rangle^{(2,a)}$	$\langle 8sF_F z 7sF_I \rangle^{(hf)}$	κ_{hf}
4-4	3.092[−11]	3.472[−13]	1.123[−02]
4-5	1.016[−10]	1.069[−12]	1.053[−02]
5-4	9.224[−11]	9.645[−13]	1.046[−02]
5-5	3.426[−11]	3.846[−13]	1.123[−02]

for calculation of the sums in Eq. (B14).

Results of our RPA calculations for the 7s-8s transitions in Fr are presented in Table II. The state dependence of κ_{hf} increases to 6–7 % in Fr in comparison to Cs, where differences in κ_{hf} for different transitions were 3–4 % in the RPA approximation. As in the case of Cs, the largest differences occur between transitions with $F_I=F_F$ and those with $F_F \neq F_I$; there is only 0.7% difference in κ_{hf} between the 4–5 and 5–4 transitions.

For the 4-3 and 3-4 hyperfine transitions in Cs measured by Wood *et al.* [1], an effective value $\kappa_{hf}=0.0049$ can be extracted from the RPA values listed in Table I. This value is about 40% smaller than the value $\kappa_{hf}=0.0078$ from Ref. [15] but agrees exactly with the value obtained earlier by Flambaum and Khriplovich [14]. We use our value of κ_{hf} to extract a value of κ_a from the Cs PNC experiment of Wood *et al.* [1],

$$\Delta \left[\frac{\text{Im}(E_{\text{PNC}})}{\beta} \right]_{34-43} = -0.077 \pm 0.011 \text{ mV/cm}, \quad (10)$$

where β is the vector polarizability of the transition, which has been measured in Ref. [26] with high accuracy $\beta = 27.02(8)a_0^3$. The subscripts 34 and 43 in Eq. (10) correspond to $F_F F_I$.

The spin-independent PNC amplitude $E_{\text{PNC}}^{(1)}$ in alkali-metal atoms ($j_F=j_I=1/2$) is customarily defined as

$$E_{\text{PNC}}^{(1)} = \langle j_F 1/2 | z | j_I 1/2 \rangle, \quad (11)$$

leading to the following relation between spin-dependent PNC amplitude and the corresponding spin-dependent reduced matrix elements:

$$E_{\text{PNC}}^{(\text{sd})} = \frac{\kappa}{\mathcal{A}} \langle wF_F || z || vF_I \rangle^{(2,a)}, \quad (12)$$

where the κ is defined by Eq. (5) and \mathcal{A} is an angular coefficient,

TABLE III. Comparison of contributions to spin-dependent PNC in ^{133}Cs obtained by different groups. All results are presented in terms of the coefficients κ_a , κ_2 , κ_{hf} , and their sum κ , used in the present paper.

Group	κ	κ_2	κ_{hf}	κ_a
Present	0.117(16)	0.0140 ^a	0.0049	0.098(16)
Haxton <i>et al.</i> [18,19,27]	0.112(16) ^b	0.0140	0.0078 ^c	0.090(16)
Flambaum and Murray [28]	0.112(16) ^d	0.0111 ^e	0.0071 ^f	0.092(16) ^g
Bouchiat and Piketty [15,29]		0.0084	0.0078	

^aReferences [18,19,27].

^bReference [28].

^cReference [15].

^dThe spin-dependent matrix elements from Refs. [16,17] are used.

^eShell-model value with $\sin^2\theta_w=0.23$.

^fThis value was obtained by scaling the analytical result from Ref. [14], $\kappa_{\text{hf}}=0.0049$, by a factor 1.5.

^gContains a 1.6% correction for finite nuclear size; the raw value is 0.094(16).

$$A = (-1)^{j_F + F_I + I + 1} \sqrt{6[F_I][F_F]} \begin{Bmatrix} F_F & F_I & 1 \\ j_I & j_F & I \end{Bmatrix}, \quad (13)$$

where $[F] = 2F + 1$. For the two transitions considered here, $\mathcal{A}_{43} = -\mathcal{A}_{34}$, so we may write

$$\Delta \left[\frac{\text{Im}(E_{\text{PNC}})}{\beta} \right]_{34-43} = - \frac{\kappa}{\mathcal{A}_{43}\beta} [\langle 7sF_F \| z \| 6sF_I \rangle_{34}^{(2,a)} + \langle 7sF_F \| z \| 6sF_I \rangle_{43}^{(2,a)}] \frac{e}{4\pi\epsilon_0 a_0^2}. \quad (14)$$

Combining the experimental results for $\Delta[\text{Im}(E_{\text{PNC}})/\beta]_{34-43}$ and β with our values for the spin-dependent matrix elements from Table I, we obtain $\kappa = 0.117(16)$. The uncertainty comes from the uncertainty in the experimental value on the left side of Eq. (14); the uncertainty in β is negligibly small. In Ref. [28], $\kappa = 0.112(16)$ was obtained by combining the same experimental data [1,26] with spin-dependent matrix elements from Refs. [16,17]. This value is also used in Refs. [18,19,27]. Differences with our value of κ come only from differences in $\langle 7sF_F \| z \| 6sF_I \rangle^{(2,a)}$.

Combining the effective value for κ_{hf} with the value $\kappa_2 = 0.0140$ from Ref. [18] and the value $\kappa = 0.117(16)$ obtained above leads to $\kappa_a = 0.098(16)$, which is 8% larger than the value $\kappa_a = 0.090(16)$ obtained by Haxton and Wiman [19] and 6% larger than the value $\kappa_a = 0.092(16)$ from Flambaum and Murray [28]. To clarify the sources of these differences, we compare our results with those from Refs. [15,18,19,27–29] in Table III. We scaled the constants given in [15,28,29] to represent them in terms of the coefficients κ , κ_a , κ_2 , κ_{hf} used here.

The revised value of κ_{hf} and $\langle 7sF_F \| z \| 6sF_I \rangle^{(2,a)}$ obtained in this work increases the value of the ^{133}Cs anapole moment, and thereby slightly increases the differences between various experimental constraints on PNC meson coupling constants discussed in Ref. [19]. Since correlation corrections to $\langle 7sF_F \| z \| 6sF_I \rangle^{(2,a)}$ are large, 25% at the RPA level, further accurate calculations are clearly desirable.

Measuring the PNC electric-dipole transition between ground-state hyperfine levels is a potentially fruitful method for obtaining experimental anapole moments for atoms other than Cs. Schemes have been proposed to carry out such measurements and calculations have been carried out for various atoms in Refs. [30–34]. The contribution of the spin-independent interaction from Z exchange, which dominates the PNC dipole matrix element between different atomic levels, vanishes for the microwave transitions between hyperfine states of the same level.

As an aid to the analysis of these microwave experiments, we give reduced matrix elements $\langle F_F \| z \| F_I \rangle^{(2,a)}$ induced by the spin-dependent interaction of Eq. (1) together with values of the third-order dipole matrix element $\langle F_F \| z \| F_I \rangle^{(\text{hf})}$ for atoms of potential experimental interest in Table IV. The corresponding calculations were carried out at the RPA level of approximation. The ratio of matrix elements again gives κ_{hf} . The ground-state configurations of the atoms listed in the table are $ns_{1/2}$ or $np_{1/2}$, and the hyperfine levels have angular momentum $F = I \pm 1/2$. For some of the atoms considered in Table IV, RPA correlation corrections to the weak-hyperfine interference matrix element are no longer small; they contribute 20% and 34% to $\langle F_F \| z \| F_I \rangle^{(\text{hf})}$ for Au and Ra^+ , respectively.

IV. SUMMARY

We have considered the PNC dipole matrix elements induced by the combined hyperfine-weak interaction and found that they are, at the few percent level of accuracy, proportional to the PNC dipole matrix elements induced by the spin-dependent interaction of Eq. (1), independent of F_I and F_F , for transitions $F_I - F_F$ between hyperfine levels. The proportionality is not the result of an operator identity, but of similar angular-momentum structures for the respective matrix elements. By carrying out calculations at the RPA level of approximation, which are expected to be accurate to a few percent, we are able to extract effective coupling constants κ_{hf} from the calculations. Although the dominant matrix element $\langle wIF_F \| z \| vIF_I \rangle^{(2,a)}$ is sensitive to correlation corrections, increasing by 10–30% in Cs and Fr when correlation corrections are included, the matrix element

TABLE IV. We list values of κ_{hf} for microwave transitions between ground-state hyperfine levels F_F-F_I in atoms of potential experimental interest. In this table, A is the atomic number, I is the nuclear spin, μ_I is the nuclear moment, Q_W is the weak charge (including radiative corrections), C is the 50% falloff radius of both the nuclear $\rho(r)$ and magnetization $M(r)$ distributions (the 10%–90% falloff distance is taken as 2.3 fm). The ground-state configurations of the atoms considered here are $ns_{1/2}$ or $np_{1/2}$ and the hyperfine levels have angular momentum $F=I\pm 1/2$. The PNC reduced dipole matrix elements induced by the spin-dependent Hamiltonian of Eq. (1), $\langle F_F||z||F_I\rangle^{(2,a)}$, are given together with the third-order dipole matrix elements $\langle F_F||z||F_I\rangle^{(\text{hf})}$; their ratio gives κ_{hf} . These calculations are carried out at the RPA level of approximation. Numbers in square brackets represent powers of 10.

Atom	A	I	μ_I	Q_W	$C(\text{fm})$	nl	F_F-F_I	$\langle F_F z F_I\rangle^{(2,a)}$	$\langle F_F z F_I\rangle^{(\text{hf})}$	κ_{hf}
K	39	3/2	0.39149	-18.39	3.611	$4s$	1-2	-2.222[-13]	-1.113[-16]	5.01[-04]
K	41	3/2	0.21448	-20.36	3.611	$4s$	1-2	-2.222[-13]	-6.753[-17]	3.04[-04]
Rb	85	5/2	1.3534	-44.75	4.871	$5s$	2-3	-2.550[-12]	-5.432[-15]	2.13[-03]
Rb	87	3/2	2.7515	-46.73	4.871	$5s$	1-2	-1.363[-12]	-1.027[-14]	7.54[-03]
Cs	133	7/2	2.5826	-73.09	5.675	$6s$	3-4	-1.724[-11]	-7.791[-14]	4.52[-03]
Ba ⁺	135	3/2	0.83863	-74.01	5.721	$6s$	1-2	-6.169[-12]	-2.217[-14]	3.59[-03]
Ba ⁺	137	3/2	0.93735	-75.98	5.721	$6s$	1-2	-6.169[-12]	-2.544[-14]	4.12[-03]
Au	197	3/2	0.14816	-110.88	6.554	$6s$	1-2	-1.601[-11]	-1.912[-14]	1.19[-03]
Tl	203	1/2	1.6222	-114.69	6.618	$6p_{1/2}$	0-1	-3.000[-11]	-3.437[-13]	1.15[-02]
Tl	205	1/2	1.6382	-116.66	6.618	$6p_{1/2}$	0-1	-3.000[-11]	-3.531[-13]	1.18[-02]
Fr	211	9/2	4.00	-116.23	6.733	$7s$	4-5	-2.379[-10]	-2.223[-12]	9.34[-03]
Fr	223	3/2	1.17	-128.08	6.834	$7s$	1-2	-5.820[-11]	-5.187[-13]	8.91[-03]
Ra ⁺	223	3/2	0.2705	-127.02	6.866	$7s$	1-2	-5.987[-11]	-1.258[-13]	2.10[-03]

$\langle wIF_F||z||vIF_I\rangle^{(\text{hf})}$ is correlation insensitive, changing by less than 6% for these cases.

For the case of ^{133}Cs , the value of κ_{hf} is about 40% smaller than that obtained in an earlier calculation [15] and slightly increases the size of the anapole moment of ^{133}Cs inferred from experiment [1,19]. Values of κ_{hf} are also presented for the $7s$ - $8s$ transition in Fr and for microwave transitions between ground-state hyperfine levels in atoms of potential experimental interest.

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APPENDIX A: THIRD-ORDER PERTURBATION THEORY

We introduce a perturbation $V_I=H^{(1)}+H^{(\text{hf})}$ into the many-body Hamiltonian H_0 describing an atom and expand the many-body wave function Ψ of the bound state v in powers of V_I ,

$$\Psi = \Psi_v + \Psi_v^{(1)} + \Psi_v^{(2)} + \dots,$$

to find

$$\Psi_v^{(1)} = \sum_{n \neq v} \frac{|n\rangle \langle n|V_I|v\rangle}{E_v - E_n}, \quad (\text{A1})$$

$$\begin{aligned} \Psi_v^{(2)} = & -\frac{1}{2} \sum_{n \neq v} \frac{\langle v|V_I|n\rangle \langle n|V_I|v\rangle}{(E_v - E_n)^2} \psi_v \\ & - E_v^{(1)} \sum_{m \neq v} \frac{|m\rangle \langle m|V_I|v\rangle}{(E_v - E_m)^2} \\ & + \sum_{\substack{m \neq v \\ n \neq v}} \frac{|m\rangle \langle m|V_I|n\rangle \langle n|V_I|v\rangle}{(E_v - E_m)(E_v - E_n)}, \end{aligned} \quad (\text{A2})$$

where

$$E_v^{(1)} = \langle v|V_I|v\rangle \equiv \langle v|H^{(\text{hf})}|v\rangle \quad (\text{A3})$$

is the first-order correction to the energy. The approximate wave function $\Psi_v + \Psi_v^{(1)} + \Psi_v^{(2)}$ is normalized to second order.

The third-order matrix element of the dipole operator is given by

$$\langle w|z|v\rangle^{(3)} = \langle \Psi_w^{(2)}|z|\Psi_v\rangle + \langle \Psi_w^{(1)}|z|\Psi_v^{(1)}\rangle + \langle \Psi_w|z|\Psi_v^{(2)}\rangle. \quad (\text{A4})$$

Expanding this expression, we obtain

$$\begin{aligned}
\langle w|z|v\rangle^{(3)} = & -\frac{1}{2} \sum_{m \neq w} \frac{\langle w|V_I|m\rangle\langle m|V_I|w\rangle}{(E_w - E_m)^2} \langle w|z|v\rangle - E_w^{(1)} \sum_{m \neq w} \frac{\langle w|V_I|m\rangle\langle m|z|v\rangle}{(E_w - E_m)^2} + \sum_{\substack{m \neq w \\ n \neq w}} \frac{\langle w|V_I|n\rangle\langle n|V_I|m\rangle\langle m|z|v\rangle}{(E_w - E_m)(E_w - E_n)} \\
& + \sum_{\substack{m \neq w \\ n \neq v}} \frac{\langle w|V_I|m\rangle\langle m|z|n\rangle\langle n|V_I|v\rangle}{(E_w - E_m)(E_v - E_n)} - \frac{1}{2} \sum_{n \neq v} \frac{\langle v|V_I|n\rangle\langle n|V_I|v\rangle}{(E_v - E_n)^2} \langle w|z|v\rangle - E_v^{(1)} \sum_{n \neq v} \frac{\langle w|z|n\rangle\langle n|V_I|v\rangle}{(E_v - E_n)^2} \\
& + \sum_{\substack{m \neq v \\ n \neq v}} \frac{\langle w|z|n\rangle\langle n|V_I|m\rangle\langle m|V_I|v\rangle}{(E_v - E_m)(E_v - E_n)}. \tag{A5}
\end{aligned}$$

Setting $V_I = H^{(1)} + H^{(\text{hf})}$ and retaining only those terms linear in $H^{(1)}$, we obtain the expression given in Eq. (9). It should be noted that the two terms above proportional to $\langle w|z|v\rangle$ do not contribute when the states v and w have the same parity.

APPENDIX B: ANGULAR DECOMPOSITION

The matrix element of the spin-independent operator $H^{(1)}$ between single-particle states $|i\rangle$ and $|j\rangle$ is

$$\begin{aligned}
\langle i|H^{(1)}|j\rangle = & i \frac{G}{2\sqrt{2}} Q_w \delta_{\kappa_i - \kappa_j} \delta_{m_i m_j} \int_0^\infty dr [F_i(r) G_j(r) \\
& - G_i(r) F_j(r)] \rho(r). \tag{B1}
\end{aligned}$$

Here, (κ_i, m_i) are angular-momentum quantum numbers of the state $|i\rangle$ [$\kappa_i = \mp(j_i + 1/2)$, for $j_i = l_i \pm 1/2$], l_i and j_i being the orbital and the total angular momentum, respectively, of the state $|i\rangle$. The functions $G_i(r)$ and $F_i(r)$ are the large and small radial components, respectively, of the Dirac wave function for the state $|i\rangle$. We define the reduced matrix element of $H^{(1)}$ as the coefficient of the angular-momentum deltas in Eq. (B1). Using this (somewhat unconventional) definition, it follows that

$$\begin{aligned}
\langle i||H^{(1)}||j\rangle = & i \frac{G}{2\sqrt{2}} Q_w \int_0^\infty dr [F_i(r) G_j(r) \\
& - G_i(r) F_j(r)] \rho(r). \tag{B2}
\end{aligned}$$

We decompose the spin-dependent operators of the type $H^{(k)}$, with $k = (a, 2)$ in a spherical basis as

$$H^{(k)} = \sum_{\mu} (-1)^{\mu} I_{-\mu} K_{\mu}^{(k)}.$$

(In this equation, we omit the multiplicative factors κ_a and κ_2 defined in Sec. I to avoid confusion with the angular-momentum quantum numbers κ_i introduced in the previous paragraph.) The matrix element of the purely electronic operator $K_{\mu}^{(k)}$ between single-particle states $|i\rangle$ and $|j\rangle$ is

$$\begin{aligned}
\langle i|K_{\mu}^{(k)}|j\rangle = & i \frac{G}{\sqrt{2}} \int_0^\infty dr \rho(r) [\langle -\kappa_i m_i | \sigma_{\mu} | \kappa_j m_j \rangle F_i(r) G_j(r) \\
& - \langle \kappa_i m_i | \sigma_{\mu} | -\kappa_j m_j \rangle G_i(r) F_j(r)]. \tag{B3}
\end{aligned}$$

From this, it follows

$$\begin{aligned}
\langle i||K^{(k)}||j\rangle = & i \frac{G}{\sqrt{2}} \int_0^\infty dr \rho(r) [\langle -\kappa_i || \sigma || \kappa_j \rangle F_i(r) G_j(r) \\
& - \langle \kappa_i || \sigma || -\kappa_j \rangle G_i(r) F_j(r)]. \tag{B4}
\end{aligned}$$

Reduced matrix elements of the operator σ are given by

$$\langle -\kappa_i || \sigma || \kappa_j \rangle = (-1)^{j_i + \bar{l}_i - 1/2} \sqrt{6[j_i][j_j]} \delta_{\bar{l}_i \bar{l}_j} \begin{Bmatrix} j_j & j_i & 1 \\ 1/2 & 1/2 & \bar{l}_i \end{Bmatrix}, \tag{B5}$$

$$\langle \kappa_i || \sigma || -\kappa_j \rangle = (-1)^{j_i + l_i - 1/2} \sqrt{6[j_i][j_j]} \delta_{l_i \bar{l}_j} \begin{Bmatrix} j_j & j_i & 1 \\ 1/2 & 1/2 & l_j \end{Bmatrix}. \tag{B6}$$

In the above, we have used the notation $\bar{l} = l(-\kappa)$ and $[j] = 2j + 1$.

The hyperfine operator is decomposed as

$$H^{(\text{hf})} = \sum_{\lambda} (-1)^{\lambda} t_{\lambda} \mu_{-\lambda},$$

where $\mu_{\lambda} = g_I \mu_N I_{\lambda}$ is the nuclear magnetic-moment operator, and t_{λ} is the electronic part of the hyperfine interaction. We may write the reduced matrix element of the magnetic-moment operator in the nuclear ground state as

$$\langle I || \mu || I \rangle = \sqrt{I(I+1)(2I+1)} g_I \mu_N. \tag{B7}$$

In the following, the factor μ_N is absorbed into the hyperfine interaction energy scale factor:

$$W_{\text{hf}} = \frac{|e|}{4\pi\epsilon_0} \frac{|e|\hbar}{2M_p} \frac{1}{ca_0^2} = 1.987\,131 \times 10^{-6} \text{ a.u.}$$

The electronic part of the hyperfine interaction for a point nucleus in these units is given by

$$t_\lambda = -i\sqrt{2} \frac{\boldsymbol{\alpha} \cdot \mathbf{C}_{1\lambda}^{(0)}(\hat{r})}{r^2}, \quad (\text{B8})$$

where $\mathbf{C}_{1\lambda}^{(0)}(\hat{r})$ is a normalized vector spherical harmonic [[35], p. 210]. For a distributed nuclear magnetization $\mathbf{M}(r)$, Eq. (B8) becomes

$$t_\lambda = -i\sqrt{2} \frac{\boldsymbol{\alpha} \cdot \mathbf{C}_{1\lambda}^{(0)}(\hat{r})}{r^2} m(r), \quad (\text{B9})$$

where the function $m(r)$ is given by

$$m(r) = \frac{4\pi}{\mu} \int_0^r ds s^2 M(s) = \int_0^r ds s^2 M(s) / \int_0^\infty ds s^2 M(s).$$

For the Fermi-type distribution given in Eq. (8), we find

$$m(r, r < C) = \frac{1}{\mathcal{N}} \left[\frac{r^3}{C^3} - 3 \frac{ar^2}{C^3} S_1\left(\frac{C-r}{a}\right) + 6 \frac{a^2 r}{C^3} S_2\left(\frac{C-r}{a}\right) - 6 \frac{a^3}{C^3} S_3\left(\frac{C-r}{a}\right) + 6 \frac{a^3}{C^3} S_3\left(\frac{C}{a}\right) \right] \quad (\text{B10})$$

and

$$m(r, r > C) = 1 - \frac{1}{\mathcal{N}} \left[3 \frac{ar^2}{C^3} S_1\left(\frac{r-C}{a}\right) + 6 \frac{a^2 r}{C^3} S_2\left(\frac{r-C}{a}\right) + 6 \frac{a^3}{C^3} S_3\left(\frac{r-C}{a}\right) \right], \quad (\text{B11})$$

where \mathcal{N} is

$$\mathcal{N} = \left[1 + \frac{a^2}{C^2} \pi^2 + 6 \frac{a^3}{C^3} S_3\left(\frac{C}{a}\right) \right].$$

In the previous three equations,

$$S_k(x) = \sum_1^\infty \frac{(-1)^{n-1}}{n^k} e^{-nx}.$$

The reduced matrix element of the hyperfine operator t is

$$\begin{aligned} \langle j \| t \| i \rangle &= (\kappa_j + \kappa_i) \langle -\kappa_j \| C_1 \| \kappa_i \rangle \int_0^\infty \frac{dr}{r^2} [G_j(r) F_i(r) \\ &\quad + F_j(r) G_i(r)] m(r), \end{aligned} \quad (\text{B12})$$

where $C_{kq}(\hat{r})$ is a normalized spherical harmonic. Finally, we note that the reduced matrix element of the dipole operator z is

$$\langle j \| z \| i \rangle = \langle \kappa_j \| C_1 \| \kappa_i \rangle \int_0^\infty dr r [G_j(r) G_i(r) + F_j(r) F_i(r)]. \quad (\text{B13})$$

With the aid of the above expressions, the reduced third-order matrix element corresponding to Eq. (9) is found to be

$$\begin{aligned} \langle w I F_w \| z \| v I F_v \rangle^{(\text{hf})} &= g_I \sqrt{I(I+1)(2I+1)} [F_v] [F_w] \left(\sum_{j \neq v} (-1)^{j_v - j_w + 1} \begin{Bmatrix} F_w & F_v & 1 \\ j_j & j_w & I \end{Bmatrix} \begin{Bmatrix} I & I & 1 \\ j_j & j_v & F_v \end{Bmatrix} \right. \\ &\quad \times \left[\sum_i \frac{\langle w \| H^{(1)} \| i \rangle \langle i \| z \| j \rangle \langle j \| t \| v \rangle}{(\epsilon_j - \epsilon_v)(\epsilon_i - \epsilon_w)} + \sum_i \frac{\langle w \| z \| i \rangle \langle i \| H^{(1)} \| j \rangle \langle j \| t \| v \rangle}{(\epsilon_j - \epsilon_v)(\epsilon_i - \epsilon_w)} + \sum_i \frac{\langle w \| z \| j \rangle \langle j \| t \| i \rangle \langle i \| H^{(1)} \| v \rangle}{(\epsilon_j - \epsilon_v)(\epsilon_i - \epsilon_w)} \right. \\ &\quad \left. \left. - \frac{\langle w \| z \| j \rangle \langle j \| H^{(1)} \| v \rangle}{(\epsilon_j - \epsilon_v)^2} \langle v \| t \| v \rangle \right] + \sum_{j \neq w} (-1)^{F_v - F_w + 1} \begin{Bmatrix} F_w & F_v & 1 \\ j_v & j_j & I \end{Bmatrix} \begin{Bmatrix} I & I & 1 \\ j_j & j_w & F_w \end{Bmatrix} \right. \\ &\quad \times \left[\sum_i \frac{\langle w \| t \| j \rangle \langle j \| z \| i \rangle \langle i \| H^{(1)} \| v \rangle}{(\epsilon_i - \epsilon_v)(\epsilon_j - \epsilon_w)} + \sum_i \frac{\langle w \| H^{(1)} \| i \rangle \langle i \| t \| j \rangle \langle j \| z \| v \rangle}{(\epsilon_j - \epsilon_w)(\epsilon_i - \epsilon_w)} + \sum_i \frac{\langle w \| t \| j \rangle \langle j \| H^{(1)} \| i \rangle \langle i \| z \| v \rangle}{(\epsilon_j - \epsilon_w)(\epsilon_i - \epsilon_w)} \right. \\ &\quad \left. \left. - \langle w \| t \| w \rangle \frac{\langle w \| H^{(1)} \| j \rangle \langle j \| z \| v \rangle}{(\epsilon_j - \epsilon_w)^2} \right] \right). \end{aligned} \quad (\text{B14})$$

It is interesting to compare the interference term with the second-order reduced matrix element of the dipole operator associated with the spin-dependent terms $H^{(k)}$, $k=2,a$,

$$\begin{aligned} \langle wIF_w||z||vIF_v\rangle^{(2,a)} &= \sqrt{I(I+1)(2I+1)}[F_v][F_w] \\ &\times \sum_{j \neq v} \left[(-1)^{j_v-j_w+1} \begin{Bmatrix} F_w & F_v & 1 \\ j_j & j_w & I \end{Bmatrix} \right. \\ &\times \begin{Bmatrix} I & I & 1 \\ j_j & j_v & F_v \end{Bmatrix} \frac{\langle w||z||j\rangle\langle j||K^{(k)}||v\rangle}{\epsilon_v - \epsilon_j} \\ &+ (-1)^{F_v-F_w+1} \begin{Bmatrix} F_w & F_v & 1 \\ v & j & I \end{Bmatrix} \\ &\times \left. \begin{Bmatrix} I & I & 1 \\ j & w & F_w \end{Bmatrix} \frac{\langle w||K^{(k)}||j\rangle\langle j||z||v\rangle}{\epsilon_w - \epsilon_j} \right]. \end{aligned} \quad (\text{B15})$$

We find that the first term in this expression goes over to the first term in the interference term under the replacement

$$\begin{aligned} \langle w||z||j\rangle\langle j||K^{(k)}||v\rangle &\rightarrow g_I \left[\sum_i \frac{\langle w||H^{(1)}||i\rangle\langle i||z||j\rangle\langle j||t||v\rangle}{(\epsilon_w - \epsilon_i)} \right. \\ &+ \sum_i \frac{\langle w||z||i\rangle\langle i||H^{(1)}||j\rangle\langle j||t||v\rangle}{(\epsilon_v - \epsilon_i)} \\ &+ \sum_i \frac{\langle w||z||j\rangle\langle j||t||i\rangle\langle i||H^{(1)}||v\rangle}{(\epsilon_v - \epsilon_i)} \\ &\left. - \frac{\langle w||z||j\rangle\langle j||H^{(1)}||v\rangle}{(\epsilon_v - \epsilon_j)} \langle v||t||v\rangle \right], \end{aligned} \quad (\text{B16})$$

and that a similar correspondence can be made for the second term. The completely different dependence on the intermediate state j on the two sides of the above expression explains the state dependence of the coefficient κ_{hf} .

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