

Relations between matrix elements of different weak interactions and interpretation of the parity-nonconserving and electron electric-dipole-moment measurements in atoms and molecules

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The relations between matrix elements of different (P,T)-odd weak interactions are derived. We demonstrate that similar relations hold for parity-nonconserving transition amplitudes and electron electric dipole moments (EDMs) of atoms and molecules. This allows one to express P - and T -odd effects in many-electron systems caused by different symmetry-breaking mechanisms via each other using simple analytical formulas. We use these relations for the interpretation of the anapole moment measurements in cesium and thallium and for the analysis of the relative contributions of the scalar-pseudoscalar CP -odd weak interaction and electron EDMs to the EDMs of Cs, Tl, Fr, and other atoms and many polar molecules (YbF, PbO, ThO, etc.). Model-independent limits on electron EDMs and the parameter of the scalar-pseudoscalar CP -odd interaction are found from the analysis of the EDM measurements for Tl and YbF.

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I. INTRODUCTION

The study of the parity and time invariance violation in atoms, molecules, and nuclei is a low-energy, relatively inexpensive alternative to the high-energy search for new physics beyond the standard model (see, e.g., a review [1]). Accurate measurements of the parity nonconservation (PNC) in atoms is one of the most promising ways of exploring this path. It culminated in very precise measurements of the PNC in cesium [2]. Interpretation of the measurements based on accurate atomic calculations led to perfect agreement with the standard model and put strong constraints on any new physics beyond it [3,4] (see also review [1] for more detailed discussion). First unambiguous measurement of the nuclear P -odd *anapole moment* was also reported in the Cs PNC experiment [2].

At present, the study of symmetry violations in atoms and molecules goes mostly in three major directions (see, e.g., [5]): (i) the PNC measurements for a chain of isotopes; (ii) the measurements of nuclear anapole moments; and (iii) the measurements of the (P,T)-odd permanent electric dipole moments of atoms and molecules. Interpretation of the anapole moment and electric dipole moment (EDM) measurements requires sophisticated atomic or molecular calculations. The calculations are difficult and sometimes disagree with each other. For example, the calculations of the thallium EDM by Nataraj *et al.* [6] and by Sahoo *et al.* [7] disagree with earlier calculations [8,9], calculations of the nuclear spin-dependent PNC in cesium by Mani and Angom [10] disagree with earlier calculations [11–14], etc. The difficulties are mostly due to the strong interelectron correlations which need to be treated to all orders of the many-body perturbation theory. The majority of publications present the effect of one particular P - or CP -odd interaction for a specific atom or a molecule. If another weak interaction Hamiltonian is considered, the calculations are to be done again.

The extraction of the nuclear anapole moment from the PNC measurements for thallium [15] also presents a problem. The analysis of the experimental data based on atomic calculations

favors a negative value for the thallium anapole moment [15,16] while all nuclear calculations produce positive values [17].

Since the analysis based on sophisticated atomic calculations is very complicated it is important to have additional tools which may help to check the calculations for consistency or even avoid the calculations. In the present paper we build such tools by studying the relations between matrix elements for different symmetry-breaking operators. We show that using these relations the result for a specific operator can be easily obtained analytically if the calculations for another operator are available. The relations can also be used to check different calculations for consistency. Additional benefit comes from the need to separate the effects of different sources to the PNC or EDMs of atoms or molecules in the analysis of the experimental data. Recent measurements of T and P violation in a YbF molecule [18] combined with the Tl EDM measurement [19] would allow one to obtain independent limits on electron EDM and CP -violating interaction. However, the relative sign of these contributions is different in different calculations [9,20]. This sign problem is solved in the present work by calculating the ratio of the matrix elements. Then independent limits on electron EDMs and scalar-pseudoscalar CP -odd interaction are presented.

There is an active search for the CP -violating permanent EDMs of polar molecules, such as YbF [18], PbO [21,22], ThO [23], etc. Interpretation of the measurements requires complicated molecular calculations. Most of the calculations consider only one possible source of the molecular EDM: electron EDMs or scalar-pseudoscalar CP -odd interaction. We show that the analytical ratios of the matrix elements provide a reliable link between molecular EDMs caused by different sources. Therefore, if calculations exist for a particular CP -odd operator, no new calculations are needed to find an EDM caused by a different operator.

The approach developed in this paper is easy to apply when matrix elements of the symmetry-breaking operator between $s_{1/2}$ and $p_{1/2}$ single-electron states strongly dominate over other matrix elements. This is the case for the PNC amplitudes

between atomic s states and for the EDM of atoms and molecules caused by electron EDM or scalar-pseudoscalar CP -odd weak interaction. We also use this approach for the thallium anapole sign problem.

II. SINGLE-ELECTRON MATRIX ELEMENTS OF WEAK INTERACTION AND MANY-BODY EFFECTS

The PNC amplitude of an electric dipole transition between states of the same parity $|a\rangle$ and $|b\rangle$ is equal to

$$E1_{ba}^{\text{PNC}} = \sum_n \left[\frac{\langle b|\mathbf{d}|n\rangle\langle n|H_{\text{PNC}}|a\rangle}{E_a - E_n} + \frac{\langle b|H_{\text{PNC}}|n\rangle\langle n|\mathbf{d}|a\rangle}{E_b - E_n} \right], \quad (1)$$

where $\mathbf{d} = -e \sum_i \mathbf{r}_i$ is the electric dipole operator and H_{PNC} is the operator of a P -odd CP -even weak interaction.

The EDM of an atom in state a is given by

$$d_a = 2 \sum_n \frac{\langle a|\mathbf{d}|n\rangle\langle n|H_{CP}|a\rangle}{E_a - E_n}, \quad (2)$$

where H_{CP} is the operator of a CP -odd weak interaction.

States a , b , and n in Eqs. (1) and (2) are the many-electron atomic states. However, we can start for simplicity from an atom with one external electron above closed shells, keeping in mind the cesium atom as an example. Then in the lowest order of the perturbation theory in residual Coulomb interaction the PNC amplitude and the EDM of the atom are given by Eqs. (1) and (2) in which states a , b , and n are single-electron (e.g., Hartree-Fock) states. It is easy to see that all single-electron matrix elements of weak interaction are proportional to each other. Indeed, only short distances contribute to the value of the matrix elements (see the Appendix for analytical estimations). These distances are $r < r_N$ for the PNC interactions and for the scalar-pseudoscalar CP -odd interaction (r_N is nuclear radius) and $r \leq a_0/Z$ for the electron EDM operator (a_0 is Bohr radius). On these distances the energy of the single-electron state can be neglected compared to the nuclear potential $-Ze^2/r$ and Dirac equations for all single-electron states become identical. The only difference comes from the normalization of the states. Suppose we have two different operators of, say, CP -odd weak interaction H_{CP} and H'_{CP} . If we establish proportionality between matrix elements for a particular pair i, j of single-electron states

$$\langle i|H_{CP}|j\rangle = R\langle i|H'_{CP}|j\rangle, \quad (3)$$

then due to the proportionality of the wave functions on short distances, the same proportionality, with the same value of R would hold for any pair of single-electron states and for the total EDM of atom (2). Furthermore, if the $s_{1/2}$ - $p_{1/2}$ matrix elements of the weak interaction strongly dominate over other matrix elements, then the proportionality is not affected by the many-body effects. Indeed, if other weak matrix elements are neglected, then any many-body expression is a sum of terms with one $s_{1/2}$ - $p_{1/2}$ weak matrix element in each term. Since all of them are proportional with the same proportionality coefficient R the proportionality would hold for the sum as well.

Table I shows the ratios of the $\langle 6s_{1/2}|H_W|6p_{1/2}\rangle$ matrix elements for a cesium atom for different P -odd and CP -

TABLE I. The ratio of the matrix elements of the spin-dependent to spin-independent P -odd weak interactions (R_1) and scalar-pseudoscalar CP -odd interaction to electron EDMs (R_2) for the $6s, 6p_{1/2}$ states of cesium with and without the inclusion of dominating many-body effects. The ratios are stable whereas the matrix elements change by up to two times. Units: $\varkappa/(-Q_W)$ for R_1 and $10^{-15} C^{\text{SP}}/d_e$ a.u. for R_2 .

Approximation		R_1	R_2
RHF	$\langle \psi_{6s}^{\text{HF}} H_W \psi_{6p}^{\text{HF}}\rangle$	4.78	8.96
RPA	$\langle \psi_{6s}^{\text{HF}} H_W + \delta V_{\text{core}} \psi_{6p}^{\text{HF}}\rangle$	4.88	8.94
BO ^a	$\langle \psi_{6s}^{\text{BO}} H_W \psi_{6p}^{\text{BO}}\rangle$	4.78	9.03
BO + CP^b	$\langle \psi_{6s}^{\text{BO}} H_W + \delta V_{\text{core}} \psi_{6p}^{\text{BO}}\rangle$	4.85	9.01
Analytical, Eqs. (A10), (A13), and (A15)		4.84	9.01

^aBrueckner orbitals.

^bBrueckner orbitals and core polarization.

odd operators of weak interaction H_W in the relativistic Hartree-Fock (RHF) approximation and with dominating many-body effects included. The ratios are compared with the analytical result presented in the Appendix. The many-body effects include core-polarization (CP) and Brueckner-type correlations. Core polarization can be understood as the change of the self-consistent core potential due to the effect of an external field (weak interaction in our case). Its inclusion above the Hartree-Fock level is often called the *random-phase approximation* (RPA). Brueckner-type correlations are the correlations which can be reduced to a redefinition of the single-electron orbitals, replacing the Hartree-Fock ones by the Brueckner orbitals (BO) [24]. In both cases of the P -odd and CP -odd weak interactions the ratios of the matrix elements are stable within 1–2 % accuracy whereas the matrix elements change by up to two times.

III. PARITY NONCONSERVATION

A Hamiltonian describing a parity-nonconserving electron-nuclear interaction can be written as a sum of spin-independent (SI) and spin-dependent (SD) parts (we use atomic units: $\hbar = |e| = m_e = 1$):

$$H_{\text{PNC}} = H_{\text{SI}} + H_{\text{SD}} = \frac{G_F}{\sqrt{2}} \left(-\frac{Q_W}{2} \gamma_5 + \frac{\varkappa}{I} \boldsymbol{\alpha} \mathbf{I} \right) \rho(\mathbf{r}), \quad (4)$$

where $G_F \approx 2.2225 \times 10^{-14}$ a.u. is the Fermi constant of the weak interaction, Q_W is the nuclear weak charge, $\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}$

and $\gamma_5 = \begin{pmatrix} 0 & -I \\ -I & 0 \end{pmatrix}$ are Dirac matrices, \mathbf{I} is the nuclear spin, and $\rho(\mathbf{r})$ is the nuclear density normalized to 1. The strength of the spin-dependent PNC interaction is proportional to the dimensionless constant \varkappa which is to be found from the measurements. There are three major contributions to \varkappa arising from (i) electromagnetic interaction of atomic electrons with nuclear anapole moment [25], (ii) electron-nucleus spin-dependent weak interaction [26], and (iii) a combined effect of the spin-independent weak interaction and the magnetic hyperfine interaction [27] (see also review [1]). In this work we do not distinguish between different contributions to \varkappa and present the results in terms of total \varkappa which is the sum of all possible contributions.

Within the standard model the weak nuclear charge Q_W is given by [28]

$$Q_W \approx -0.9877N + 0.0716Z. \quad (5)$$

Here N is the number of neutrons and Z is the number of protons.

The PNC amplitude of an electric dipole transition between states of the same parity $|i\rangle \equiv |J_i F_i M_i\rangle$ and $|f\rangle \equiv |J_f F_f M_f\rangle$ is equal to

$$E1_{fi}^{\text{PNC}} = \sum_n \left[\frac{\langle f | \mathbf{d} | n \rangle \langle n | H_{\text{PNC}} | i \rangle}{E_i - E_n} + \frac{\langle f | H_{\text{PNC}} | n \rangle \langle n | \mathbf{d} | i \rangle}{E_f - E_n} \right], \quad (6)$$

where $\mathbf{d} = -e \sum_i \mathbf{r}_i$ is the electric dipole operator and $\mathbf{F} = \mathbf{I} + \mathbf{J}$ is the total angular momentum.

Applying the Wigner-Eckart theorem we can express the amplitudes via reduced matrix elements

$$E1_{fi}^{\text{PNC}} = (-1)^{F_f - M_f} \begin{pmatrix} F_f & 1 & F_i \\ -M_f & q & M_i \end{pmatrix} \langle J_f F_f || d_{\text{PNC}} || J_i F_i \rangle. \quad (7)$$

Detailed expressions for the reduced matrix elements of the SI and SD PNC amplitudes can be found, e.g., in Refs. [29] and [30]. For the SI amplitude we have

$$\begin{aligned} & \langle J_f, F_f || d_{\text{SI}} || J_i, F_i \rangle \\ &= (-1)^{I + F_i + J_f + 1} \sqrt{(2F_f + 1)(2F_i + 1)} \begin{Bmatrix} J_i & J_f & 1 \\ F_f & F_i & I \end{Bmatrix} \\ & \times \sum_n \left[\frac{\langle J_f || \mathbf{d} || n, J_n \rangle \langle n, J_n | H_{\text{SI}} | J_i \rangle}{E_i - E_n} \right. \\ & \left. + \frac{\langle J_f | H_{\text{SI}} | n, J_n \rangle \langle n, J_n || \mathbf{d} || J_i \rangle}{E_f - E_n} \right]. \end{aligned} \quad (8)$$

It is convenient to present the amplitude in a compact form:

$$\langle J_f, F_f || d_{\text{SI}} || J_i, F_i \rangle = C(S_1 + S_2), \quad (9)$$

where $C \equiv C(F_f, J_f, F_i, J_i)$ is the angular coefficient and sums S_1 and S_2 do not depend on F_f and F_i :

$$\begin{aligned} S_1 &= \sum_n \frac{\langle J_f || \mathbf{d} || n, J_n \rangle \langle n, J_n | H_{\text{SI}} | J_i \rangle}{E_i - E_n}, \\ S_2 &= \sum_n \frac{\langle J_f | H_{\text{SI}} | n, J_n \rangle \langle n, J_n || \mathbf{d} || J_i \rangle}{E_f - E_n}. \end{aligned}$$

For the SD PNC amplitude we have

$$\begin{aligned} & \langle J_f, F_f || d_{\text{SD}} || J_i, F_i \rangle \\ &= \sqrt{(I + 1)(2I + 1)(2F_i + 1)(2F_f + 1)/I} \\ & \times \sum_n \left[(-1)^{J_f - J_i} \begin{Bmatrix} J_n & J_i & 1 \\ I & I & F_i \end{Bmatrix} \begin{Bmatrix} J_n & J_f & 1 \\ F_f & F_i & I \end{Bmatrix} \right. \\ & \left. \times \frac{\langle J_f || \mathbf{d} || n, J_n \rangle \langle n, J_n || \mathbf{b} || J_i \rangle}{E_n - E_i} \right] \end{aligned}$$

$$\begin{aligned} & + (-1)^{F_f - F_i} \begin{Bmatrix} J_n & J_f & 1 \\ I & I & F_f \end{Bmatrix} \begin{Bmatrix} J_n & J_i & 1 \\ F_i & F_f & I \end{Bmatrix} \\ & \times \frac{\langle J_f || \mathbf{b} || n, J_n \rangle \langle n, J_n || \mathbf{d} || J_i \rangle}{E_n - E_f} \end{aligned} \quad (10)$$

where \mathbf{b} is the electron part of the SD weak interaction,

$$\mathbf{b} = \frac{G_F}{\sqrt{2}} \boldsymbol{\alpha} \rho(\mathbf{r}) \boldsymbol{\alpha}. \quad (11)$$

Like in the spin-independent PNC amplitude (8), it is convenient to present the SD amplitude in a compact form:

$$\langle J_f, F_f || d_{\text{SD}} || J_i, F_i \rangle = \sum_{i=1}^4 c_i S'_i. \quad (12)$$

Here $c_i \equiv c(F_f, J_n, F_i)$ ($i = 1, 2, 3, 4$) are angular coefficients which can be extracted from Eq. (10). Sums S'_i do not depend on F_f and F_i :

$$\begin{aligned} S'_1 &= \sum_n \frac{\langle J_f || \mathbf{d} || J_n \rangle \langle J_n || \mathbf{b} || J_i \rangle}{E_n - E_i}, \\ S'_2 &= \sum_n \frac{\langle J_f || \mathbf{d} || J'_n \rangle \langle J'_n || \mathbf{b} || J_i \rangle}{E_n - E_i}, \\ S'_3 &= \sum_n \frac{\langle J_f || \mathbf{b} || J_n \rangle \langle J_n || \mathbf{d} || J_i \rangle}{E_n - E_f}, \\ S'_4 &= \sum_n \frac{\langle J_f || \mathbf{b} || J'_n \rangle \langle J'_n || \mathbf{d} || J_i \rangle}{E_n - E_f}. \end{aligned}$$

Equation (12) has more terms than Eq. (9) due to the electron vector nature of the nuclear-spin-dependent operator.

The total PNC amplitude can be presented in a form convenient for extraction of the values of \varkappa from the PNC measurements (see, e.g. [31,32])

$$E_{\text{PNC}} = E(1 + R). \quad (13)$$

Here E is the SI PNC amplitude given by Eq. (8) and R is the ratio of the SD to SI PNC amplitudes. In this work we are mostly interested in the values of R . Using compact expressions (9) and (12) one can write

$$R = \frac{c_1 S'_1 + c_2 S'_2 + c_3 S'_3 + c_4 S'_4}{C(S_1 + S_2)}. \quad (14)$$

According to the discussion of the previous section, ratios of the SD and SI weak matrix elements do not depend on the principal quantum number n . Therefore, using the ratios

$$\begin{aligned} r_1 &= \langle J_n || \mathbf{b} || J_i \rangle / \langle J_n | H_{\text{SI}} | J_i \rangle, \\ r_2 &= \langle J'_n || \mathbf{b} || J_i \rangle / \langle J_n | H_{\text{SI}} | J_i \rangle, \\ r_3 &= \langle J_f || \mathbf{b} || J_n \rangle / \langle J_f | H_{\text{SI}} | J_n \rangle, \\ r_4 &= \langle J_f || \mathbf{b} || J'_n \rangle / \langle J_f | H_{\text{SI}} | J_n \rangle, \end{aligned} \quad (15)$$

we can get rid of the sums S'_1, S'_2, S'_3, S'_4 , involving the SD matrix elements and replace them with the SI sums S_1, S_2 :

$$\begin{aligned} R &= \frac{(c_1 r_1 + c_2 r_2) S_1 + (c_3 r_3 + c_4 r_4) S_2}{C(S_1 + S_2)} \\ &= \frac{(c_1 r_1 + c_2 r_2) S_1 / S_2 + (c_3 r_3 + c_4 r_4)}{C(S_1 / S_2 + 1)}. \end{aligned} \quad (16)$$

The only parameter in Eq. (14) which comes from numerical calculations is the ratio S_1/S_2 of two different contributions to the SI PNC amplitude [see Eqs. (8) and (9)]. All other parameters are given by analytical expressions. The c_1, c_2, c_3, c_4 , and C parameters are just angular coefficients. The ratios r_1, r_2, r_3 , and r_4 can also be approximated by analytical expressions which will be discussed below.

The expression (14) can be further simplified in an important case of an $ns-n's$ transition (e.g., the $6s-7s$ transition in Cs). On a few percent level of accuracy the $s-p_{3/2}$ matrix elements of the SD PNC interaction can be neglected [32]. This means that $r_2 = r_4 = 0$. We also have $r_1 = r_3 = r$ and Eq. (16) is reduced to

$$R = r \frac{c_1 S_1/S_2 + c_3}{C(S_1/S_2 + 1)}. \quad (17)$$

Substituting r from Eq. (A10) leads to

$$R = 4.90(1 - 0.073Z^2\alpha^2) \frac{c_1 S_1/S_2 + c_3}{C(S_1/S_2 + 1)} \frac{\varkappa}{(-Q_W)}. \quad (18)$$

Q_W is the weak nuclear charge. As in Eq. (14) the only parameter which comes from numerical calculations is the ratio S_1/S_2 . On the other hand, knowing the value of R for at least two hyperfine structure (hfs) components of the PNC transition is sufficient for extraction of \varkappa from the measurements.

A. PNC in cesium

Experimental values for the two different hfs components of the parity nonconserving $6s-7s$ transition in cesium are [2]

$$\begin{aligned} E_{\text{PNC}}(6s_{F=4}-7s_{F=3}) &= 1.6349(80) \text{ mV/cm}, \\ E_{\text{PNC}}(6s_{F=3}-7s_{F=4}) &= 1.5576(77) \text{ mV/cm}. \end{aligned} \quad (19)$$

To extract \varkappa we use Eq. (13) and calculate R for these two transitions using Eq. (18). To do so we note that $J_f = J_i = J_n = 1/2$, $Q_W = -73.19$ [see Eq. (5)] and take $S_1/S_2 = -0.3459$ from Ref. [33]. This leads to the system of equations

$$\begin{aligned} E(1 + 0.06739\varkappa) &= 1.6349(80), \\ E(1 - 0.05937\varkappa) &= 1.5576(77). \end{aligned} \quad (20)$$

The solution for \varkappa is $\varkappa = 0.382(56)$. This result is in good agreement with the values $\varkappa = 0.393(56)$ from Ref. [11] and $\varkappa = 0.375(56)$ from Ref. [12].¹ Accurate calculations similar to what is reported in our previous work for Ba^+ , Yb^+ , and Ra^+ [32] lead to the value $\varkappa = 0.376$ which is in perfect agreement with the all-order calculations of Ref. [12]. This is an illustration of the accuracy of the analysis based on the ratio of the matrix elements. The value $\varkappa = 0.382$ coming from this analysis differs by less than 2% from the value $\varkappa = 0.376$ coming from the accurate calculations. This difference is due to two simplifications: (a) neglecting the $s-p_{3/2}$ matrix elements

of the SD weak interaction, and (b) assuming that the ratio of the matrix elements is the same for all single-electron states.

Recent relativistic coupled-cluster calculations of the nuclear spin-dependent PNC in Cs [10] report the values of the SD PNC matrix elements which are about 30% smaller than those of the all-order calculations of Ref. [12]. This is in disagreement not only with this work but with all earlier calculations of the SD PNC in cesium [11–14]. Given the proportionality of the matrix elements of the SI and SD weak interactions discussed above, the results of Ref. [10] are also in disagreement with all most accurate calculations of the SI PNC in cesium (see, e.g., [3,4,33]). The latter calculations have accuracy better than 0.5% and are used to test the standard model in Cs PNC experiments [2] where the accuracy is 0.35%.

B. Anapole moment of thallium

The value of the nuclear anapole moment of thallium, extracted from the measurements of the PNC in the $6p_{1/2}-6p_{3/2}$ transition [15] is in disagreement with the results of nuclear calculations (see, e.g., Ref. [17]). The analysis of the experimental data based on simple single-electron approximations gives the value $\varkappa_a = -0.22 \pm 0.30$ [15]. The analysis based on sophisticated many-body calculations gives a very close value of $\varkappa_a = -0.26 \pm 0.27$ [16]. On the other hand, the “best value” obtained in nuclear calculations is $\varkappa_a = 0.24$ [17]. To extract the sign of \varkappa_a from the experiment one needs the relative sign of SI and SD amplitudes. Here we show that simple analysis with the use of the analytical ratio of the matrix elements of the weak interactions supports the findings of Refs. [15,16] leaving the problem of sign disagreement unsolved.

If we keep only $s_{1/2}-p_{1/2}$ matrix elements of the weak interaction for both SI and SD interactions, then the general expression (16) can be reduced to

$$R(F, F') = r \frac{c(F, F')}{C(F, F')}, \quad (21)$$

where r is one of the ratios r_i , Eq. (15), which corresponds to the $s_{1/2}-p_{1/2}$ weak matrix elements, and $c(F, F')$ and $C(F, F')$ are corresponding angular coefficients. Comparing Eq. (13) to the parametrization used in [16] [$\mathcal{R} \equiv \text{Im}(E I_{\text{PNC}}/M1)$],

$$\mathcal{R}(F, F') = C(Z)[Q_W - 6\varkappa\xi(F, F')], \quad (22)$$

and substituting Eq. (A10) into Eq. (21), we get for the parameters ξ ,

$$\xi(F, F') = -0.817(1 - 0.073Z^2\alpha^2) \frac{c(F, F')}{C(F, F')}. \quad (23)$$

Corresponding values of ξ are compared in Table II with the results of the many-body calculations of [16]. We see that both calculations give very close results leaving no room for a sign error.

IV. EDM OF ATOMS AND MOLECULES

Table III shows the ratio of the $s_{1/2}-p_{1/2}$ matrix elements of the electron EDM operator (A15) to the scalar-pseudoscalar CP -odd operator (A13) for eight different atoms calculated using analytical formulas presented in the Appendix. The

¹Refs. [11] and [12] use different definitions of \varkappa . The conversion factors are $(I + 1/2)/(I + 1)$ for Ref. [11] and I for Ref. [12]. I is nuclear spin, $I = 7/2$ for ^{133}Cs .

TABLE II. Parameters $\xi(F, F')$ of the nuclear spin-dependent PNC amplitude in the $6p_{1/2}(F)$ - $6p_{3/2}(F')$ transitions in thallium.

F	F'	This work	Ref. [16]
0	1	0.947	1.10
1	1	-0.325	-0.462
1	2	-0.325	-0.348

results for cesium and thallium are in good agreement with the many-body calculations of Ref. [9], and the result for Yb^+ is in excellent agreement with the many-body calculations of Ref. [36] for the YbF molecule. We stress that the table compares the ratios of the single-electron matrix elements obtained with a simple analytical formula to the ratios of the EDMs obtained with sophisticated many-body calculations. These results provide an unambiguous link between the sign and value of two different contributions to the EDM of atoms and molecules which have a heavy atom from Table III.

A. EDM of polar molecules

Polar molecules have strong interatomic electric fields which enhance the effect of electron EDMs and lead to molecular EDMs which are several orders of magnitude larger than those in atomic systems. An experimental search is in progress for YbF [18], PbO [21,22], and ThO [23], while other molecules are also discussed in the literature (see, e.g., [34]). Interpretation of the measurements requires molecular calculations. Table IV shows the results of most recent or most accurate calculations for some polar molecules. More detailed data are presented for the YbF molecule for which the EDM measurements were recently reported [18]. The effects of electron EDM and scalar-pseudoscalar CP -odd interaction are considered. The results are presented in terms of the CP -odd parameters W_d and W_c ,

$$W_d = \langle \Psi_0 | H_e | \Psi_0 \rangle / d_e, \quad (24)$$

$$W_c = \langle \Psi_0 | H^{SP} | \Psi_0 \rangle / C^{SP}. \quad (25)$$

TABLE III. The ratio of the $s_{1/2}$ - $p_{1/2}$ matrix elements of the electron EDM operator (A15) to that of the scalar-pseudoscalar CP -odd operator (A13). Numerical results for EDMs of Cs, Tl, and YbF are also given for comparison. Units: $d_e / (C^{SP} 10^{-18} e \text{ cm})$. (For other isotopes $R' = A'R/A$).

Z	Atom	Ratios	
		Analytical	Numerical
37	^{85}Rb	228	
55	^{133}Cs	158	163 ^a
56	$^{138}\text{Ba}^+$	152	
70	$^{173}\text{Yb}^+$	114	115 ^b
81	^{205}Tl	89	83 ^c
82	^{208}Pb	88	
87	^{211}Fr	83	
90	^{232}Th	75	

^aCs atom, Ref. [9].^b YbF molecule, Ref. [36].^cTl atom, Ref. [9].TABLE IV. CP -odd interaction constants W_d and W_c for some polar molecules and their ratios. Effective electric field E_{eff} is presented together with W_d ($\langle H_e \rangle = W_d d_e = -\mathbf{E}_{\text{eff}} \mathbf{d}_e$). The results of present paper are shown in bold.

Molecule	E_{eff} (GV/cm)	W_d (10^{24} Hz/e cm)	W_c (kHz)	W_d/W_c ($10^{18}/e \text{ cm}$)
BaF	6.1 ^a	-3.0 ^a	-20	152
	6.4	-3.1	-21 ^b	152
	31 ^c	-15 ^c	-120 ^c	125
	19 ^d	-9.1 ^d	-82 ^d	111
	26 ^e	-12.6 ^e	-111	114
	25 ^f	-12 ^f	-104 ^f	115
	25 ^g	-12 ^g	-108 ^g	111
	25 ^h	-12.1 ^h	-106	114
	32 ^a	-15 ^a	-132	114
	23	-11	-92^b	114
HgF	95 ^a	-46 ^a	-511	90
PbF	-31 ^a	15 ^a	170	88
$\text{PbO } a(1)$	26.2 ⁱ	-13 ⁱ	-144	88
$\text{PbO } B(1)$	33 ⁱ	-16 ⁱ	-182	88
$\text{PbO } a(1)$	23 ^a	-11 ^a	-125	88
ThO	104 ^a	-50 ^a	-662	75
ThF^+	90 ^a	-44 ^a	-587	75

^aReference [34].^bReference [35].^cReference [37].^dReference [38].^eReference [39].^fReference [36].^gReference [40].^hReference [41].ⁱReference [42].

To compare with other works one should keep in mind that most of them present W_S instead of W_c , where

$$W_S = \frac{2}{k_s} \langle \Psi_0 | H^{SP} | \Psi_0 \rangle. \quad (26)$$

The constants k_s and C^{SP} of the strength of the CP -odd interaction are related by $Zk_s = AC^{SP}$. Factor 2 in the definition of W_S (26) is absent in some of the papers.

Most of the calculations of the molecular EDMs include only one of the CP -odd effects: that of the electron EDM or the scalar-pseudoscalar interaction. We use the relations between the matrix elements of the two CP -odd Hamiltonians to fill the gaps in the table. Corresponding results are shown in bold. For example, according to Ref. [34] the effect of electron EDM in the YbF molecule is $W_d = -15 \times 10^{24}$ Hz/e cm. Using the ratio $W_d/W_c = 114 \times 10^{18}/e \text{ cm}$ for Yb^+ from Table III we found that the effect of the scalar-pseudoscalar interaction is $W_c = -132$ kHz.

B. Extraction of the electron EDM and the parameter of the scalar-pseudoscalar CP -odd interaction from the EDM measurements for YbF and Tl

Recent measurements of T and P violation in the YbF molecule [18] combined with the Tl EDM measurement

[19] and the data from Table III allows one to obtain independent limits on the electron EDM and the CP -violating interaction. The values of the electron EDM extracted from the experimental data for Tl [19] and YbF [18] under assumption that there is no other contribution to atomic and molecular EDM read

$$\text{Tl} : d_e = (6.9 \pm 7.4) \times 10^{-28} e \text{ cm}, \quad (27)$$

$$\text{YbF} : d_e = (-2.4 \pm 5.7 \pm 1.5) \times 10^{-28} e \text{ cm}. \quad (28)$$

In fact, there are other contributions from the CP -odd electron-nucleus interactions. Here we consider only the scalar-pseudoscalar interaction (A11). Other contributions should be small due to the constraints obtained from the EDM measurements for mercury [43]. Using data from Table III one can rewrite Eqs. (27) and (28) as

$$\text{Tl} : d_e + 1.2 \times 10^{-20} C^{\text{SP}} = (6.9 \pm 7.4) \times 10^{-28} e \text{ cm}, \quad (29)$$

$$\text{YbF} : d_e + 8.8 \times 10^{-21} C^{\text{SP}} = (-2.4 \pm 5.7 \pm 1.5) \times 10^{-28} e \text{ cm}. \quad (30)$$

Solving these equations for d_e and C^{SP} leads to

$$d_e = (-2.8 \pm 3.0) \times 10^{-27} e \text{ cm}, \quad (31)$$

$$C^{\text{SP}} = (3.0 \pm 3.0) \times 10^{-7}. \quad (32)$$

The limit (31) for d_e is significantly weaker than those presented in Eqs. (27) and (28). This is because the values of the ratios of the matrix elements of the two operators are very close for Tl and Yb (see Table III). The most fortunate case leading to the strongest limits for d_e and C^{SP} would correspond to very different values of the ratio, preferably with the different sign. However, the formulas (A15) and (A13) and the data in Table III show that this is not possible. The ratio is always positive and slowly decreases with Z . A slightly different value of the ratio should be expected for the EDM of radium in the excited metastable $7s6d^3D_2$ state. The EDM of radium in this state is strongly enhanced [44] due to the proximity of the $7s7p^3P_1^0$ state (the energy interval is $\sim 5 \text{ cm}^{-1}$) and is proportional to the $\langle 7p_{3/2} | H_{CP} | 6d_{3/2} \rangle$ matrix element of the CP -odd interaction H_{CP} . However, the value of this matrix element is strongly dominated by the core-polarization effect which in turn is mostly due to the $s_{1/2}$ - $p_{1/2}$ matrix elements between the core and excited states. Therefore, the ratio of the two contributions is not very different from what was considered above for Tl and YbF.

C. EDM of Tl and Fr

The EDM of thallium due to electron EDMs and scalar-pseudoscalar CP -odd interaction was recently calculated in our paper [9]. The ratio of the two contributions was found to be $83d_e/(C^{\text{SP}}10^{-18}e \text{ cm})$ which is in good agreement with the analytical result of this paper: $W_d/W_e = 89/(10^{-18}e \text{ cm})$. The EDM enhancement factor is -582 [9] which is in very good agreement with the value -585 found in earlier calculations by Liu and Kelly [8]. The EDM enhancement factor for thallium was also calculated in the more recent work of Ref. [6] and found to be -466 ($d_{\text{Tl}} = -466d_e$) which is about 25% smaller than the results mentioned above. The EDM of thallium due to

the scalar-pseudoscalar CP -odd interaction calculated by the same group earlier ($d_{\text{Tl}} = -4.06 \times 10^{-18} C^{\text{SP}} e \text{ cm}$ [7]) is also smaller than in the other calculations of Refs. [9] and [20]. On the other hand, the ratio of the two contributions is 115 [in units of $d_e/(C^{\text{SP}}10^{-18}e \text{ cm})$] which is significantly larger than the analytical and numerical values of 89 and 83 (same units, see Table III).

The EDM enhancement factor for francium was calculated in Ref. [49] and found to be 910(46): $d(\text{Fr}) = 910(46)d_e$. This value is in good agreement with the value of 894.93 found in more recent calculations [50]. Using the value $d(\text{Fr}) = 910(46)d_e$ and the ratio of the electron-EDM matrix element to the scalar-pseudoscalar interaction presented in Table III we can now reconstruct another contribution to the EDM of francium:

$$d(\text{Fr}) = 11 \times 10^{-18} C^{\text{SP}} e \text{ cm}. \quad (33)$$

It is interesting to note that the calculation of the nuclear spin-dependent PNC amplitude between hyperfine components of the ground state of francium presented in Ref. [29] involves the same sum as expression (2) for the EDM of the atom. Therefore, we can reconstruct the EDM enhancement factor for Fr using the results of Ref. [29] and proportionality between matrix elements of the nuclear spin-dependent interaction (A9) and the electron EDM operator (A15). This leads to $d(\text{Fr}) = 854d_e$ which is in good agreement with the value $d(\text{Fr}) = 910(46)d_e$ of Ref. [49]. This is a good consistency test of both calculations.

Reading the papers citing our works (see, e.g., [6,50]) reveals the need to clear up some points about our method of calculations. For example, the atomic electric field interacting with electron EDMs is calculated in [9] and [49] as a derivative of the total potential which includes both nuclear and electron parts. The formula $\mathbf{E} = Z\mathbf{e}r/r^3$ for the leading contribution to the atomic electric field presented on first page of [49] may make an impression that only the nuclear field is included. However, the formula (2) a few lines below clearly includes screening functions $Q(r)$ and $P(r)$ for both the nuclear Coulomb and the external electric field. By the way, the inclusion of the electron electric field changes the matrix elements of the electron EDM for thallium by only 0.4%. This is because the main contribution comes from short distances where the electron electric field is small since the electron potential rapidly tends to a constant inside the $1s$ orbital. Therefore, we include only the nuclear electric field in the analytical analysis [formula (A15) in the Appendix] while keeping both contributions in the numerical calculations.

The authors of [6] claim that the atomic core is strongly contracted in the V^{N-3} starting approximation used in our calculations [9]. In fact, it is not. Figure 1 shows the outermost $5d_{5/2}$ core function of Tl calculated in the V^{N-3} and V^{N-1} approximations. The difference between the functions is very small. This is due to the fact that the valence $6s$ and $6p$ electrons are located outside of the atomic core. Their charge distribution creates an almost constant potential and no electric field inside the sphere where all inner electrons are located. Therefore, the valence electrons have practically no effect on the core wave functions (see [45] for a detailed discussion). The change is even smaller for other core functions. The core functions enter the configuration-interaction (CI) Hamiltonian

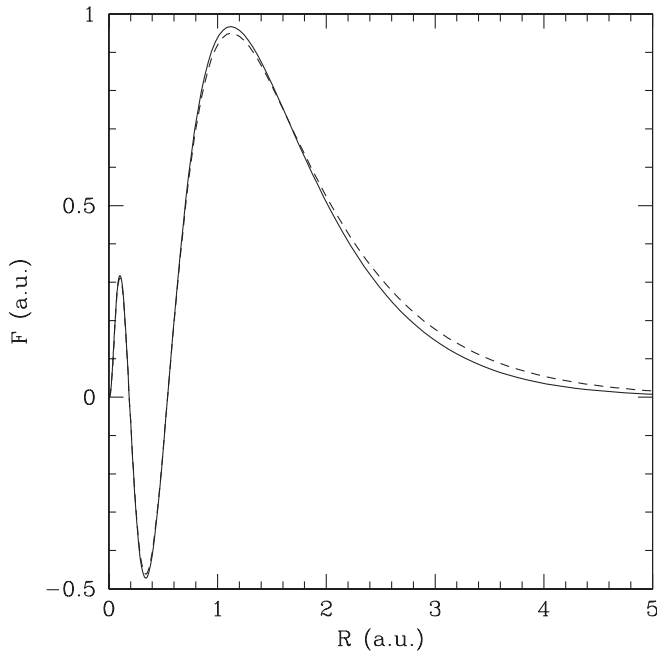


FIG. 1. The $5d_{5/2}$ core function of Tl calculated in V^{N-3} (solid line) and V^{N-1} (dashed line) approximations.

via core potential V_{core} to which all core electrons contribute (from $1s$ to $5d$). The difference for V_{core} in the V^{N-3} and V^{N-1} approximations is very small [45]. Moreover, the corresponding corrections to the CI Hamiltonian have been included in [9] using the many-body perturbation theory approach.

As is well known, the eigenstates of a Hamiltonian do not depend on the basis one uses. The valence states are indeed different in the V^{N-3} and V^{N-1} approximations. However, this should have no effect on the final results as long as the saturation of the basis for valence states is achieved. There are only two conditions the basis states must satisfy: (a) they must be orthogonal to the core, and (b) they must constitute a complete set of states. Therefore, it does not matter whether valence states are calculated in the V^{N-3} or V^{N-1} potential or by any other method [e.g., a popular basis $\psi_n(r) = r^n \psi_0(r)$ [46]], the final results should be the same. If there is any difference in the results, the most likely reason for this is the incompleteness of the basis set.

In spite of no difference in the final results there is a good reason for the use of the V^{N-3} approximation—the simplicity and good convergence of the many-body perturbation theory (MBPT) for the core-valence correlations. This is the only approximation that has no *subtraction diagrams* [47,48]. To be more precise, we should state that the condition for the absence of the subtraction diagrams is that the potential used to calculate single-electron core states and the potential of the core in the CI Hamiltonian are exactly the same. In the case of the thallium atom treated as a three-valence-electron system this corresponds to the V^{N-3} approximation. When any other approximation is used one has to include the subtraction diagrams.

Large energy denominators suppress the value of the correlation terms in the V^{N-3} approximation ensuring good convergence of the MBPT [45]. There must be large cancella-

tion between subtraction and other diagrams to ensure the same final results if any other initial approximation is used. This is very similar to the well-known fact that the Hartree-Fock basis is the best choice for any MBPT calculations. Zero-order results might be better in some other approximation, however, strong cancellation between subtraction and other diagrams would lead to poor convergence of the MBPT.

The authors of [6] claim that the major drawback of our work [9] is the inclusion of the core-valence correlations in the second order only. However, the correlations between the valence electrons and core electrons below the $6s$ state are small, which is evident from the fact that their inclusion changes the EDM of Tl by only 3% [9]. Therefore, only the correlations between three valence electrons should be treated to all orders. This is done in [9] to a very high precision using the CI technique.

V. CONCLUSION

We have demonstrated the proportionality relations between the nuclear-spin-dependent and spin-independent PNC effects in atoms and the scalar-pseudoscalar and the electron EDM contributions to the EDMs of atoms and molecules. The relations are given by the simple analytical formulas and can be used to express one symmetry-breaking effect through another. Using these relations and accurate calculations of the spin-independent PNC we have confirmed earlier interpretations of the nuclear anapole measurements in cesium and thallium. We have also confirmed the ratio of the scalar-pseudoscalar CP -odd and electron EDM contributions to the EDMs of Cs, Tl, and other atoms and some polar molecules. Using the relations we found the scalar-pseudoscalar contribution to the EDM of the francium atom and the scalar-pseudoscalar and electron EDM contributions to the EDMs of many polar molecules. Using experimental limits on the EDMs of thallium and YbF we found model-independent limits on the electron EDMs and the constant of the scalar-pseudoscalar CP -odd interaction.

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APPENDIX: MATRIX ELEMENTS OF THE WEAK INTERACTION

1. Wave function

We use single-electron wave functions in the form

$$\psi(r)_{njlm} = \frac{1}{r} \begin{pmatrix} f_v(r)\Omega(\mathbf{n})_{jlm} \\ i\alpha g_v(r)\tilde{\Omega}(\mathbf{n})_{jlm} \end{pmatrix}, \quad (\text{A1})$$

where n is the principal quantum number and an index v replaces the three-number set n, j, l ; α is the fine-structure constant.

We need $s_{1/2}$ and $p_{1/2}$ wave functions inside the nucleus to calculate matrix elements. Following Ref. [51] we assume uniform distribution of the electric charge inside a sphere of radius R_N . Taking formulas for the $s_{1/2}$ and $p_{1/2}$ wave

functions from Ref. [51] and keeping terms up to $Z^2\alpha^2$ we come to the following expressions:

$$\begin{aligned} f_s(x) &= A_s x \left(1 - \frac{3}{8} Z^2 \alpha^2 x^2\right), \\ g_s(x) &= -A_s Z \frac{x^2}{2} \left(1 - \frac{x^2}{5}\right), \\ f_{p_{1/2}}(x) &= A_p Z \alpha^2 \frac{x^2}{2} \left(1 - \frac{x^2}{5}\right), \\ g_{p_{1/2}}(x) &= A_p x \left(1 - \frac{3}{8} Z^2 \alpha^2 x^2\right). \end{aligned} \quad (\text{A2})$$

Here $x = r/R_N$, where R_N is the nuclear radius. A_s and A_p are the normalization factors. They can be found by matching Eq. (A2) to the atomic wave functions at short distances outside of the nucleus (see, e.g., [52]). The use of the semiclassical wave functions presented in [52] leads to approximate expressions

$$\begin{aligned} A_s &= \frac{(1 + \gamma)(2ZR_N)^\gamma}{(1 - 0.375Z^2\alpha^2)\sqrt{Z}\Gamma(2\gamma + 1)v_s^{1.5}}, \\ A_p &= \frac{\sqrt{Z}(2ZR_N)^\gamma}{(1 - 0.375Z^2\alpha^2)\Gamma(2\gamma + 1)v_p^{1.5}}, \end{aligned} \quad (\text{A3})$$

where $\gamma = \sqrt{1 - Z^2\alpha^2}$, Γ is the gamma function, and ν is the effective principal quantum number: the single-electron energy of state n is $\epsilon_n = -1/(2\nu_n^2)$. Note that normalization factors (A3) are needed only to compare the matrix elements of the electron EDM to other matrix elements. For cases not involving electron EDMs there is exact cancellation of the normalization factors. Therefore, their uncertainty does not contribute to the uncertainty of the final results.

2. PNC matrix elements

The matrix element of the SI PNC H_{SI} interaction [the first term in Eq. (4)] is

$$\langle \kappa_1 | H_{\text{SI}} | \kappa_2 \rangle = i \frac{G_F Q_W}{2\sqrt{2}} \alpha \delta_{-\kappa_1, \kappa_2} \int (f_1 g_2 - g_1 f_2) \rho(r) dr. \quad (\text{A4})$$

Substituting Eq. (A2) for the $s_{1/2}$ - $p_{1/2}$ transition and assuming uniform nuclear charge distribution we get

$$\langle s_{1/2} | H_{\text{SI}} | p_{1/2} \rangle = i \frac{G_F Q_W}{2\sqrt{2}} \frac{\alpha \rho_0 A_s A_p R_N}{3} (1 - 0.34Z^2\alpha^2). \quad (\text{A5})$$

Here A_s and A_p are given by Eq. (A3) and

$$\rho_0 = \frac{3}{4\pi R_N^3}. \quad (\text{A6})$$

The matrix element of the SD PNC \mathbf{b} operator (11) is

$$\begin{aligned} \langle \kappa_1 | \mathbf{b} | \kappa_2 \rangle &= -i \frac{G_F \varkappa}{\sqrt{2}} \alpha \langle -\kappa_1 | C_1 | \kappa_2 \rangle \int [(\kappa_2 - \kappa_1 + 1) f_1 g_2 \\ &\quad - (\kappa_1 - \kappa_2 + 1) g_1 f_2] \rho(r) dr. \end{aligned} \quad (\text{A7})$$

The reduced matrix element of the spherical harmonic C_k is

$$\begin{aligned} \langle \kappa_a | C_k | \kappa_b \rangle &= (-1)^{j_b+1/2} \sqrt{(2j_a+1)(2j_b+1)} \\ &\quad \times \xi(j_a + l_b + k) \begin{pmatrix} j_b & j_a & k \\ -1/2 & 1/2 & 0 \end{pmatrix}, \\ \xi(x) &= \begin{cases} 1 & x \text{ is even} \\ 0 & x \text{ is odd.} \end{cases} \end{aligned} \quad (\text{A8})$$

For the $s_{1/2}$ - $p_{1/2}$ transition and uniform nuclear charge distribution we have

$$\langle s_{1/2} | \mathbf{b} | p_{1/2} \rangle = -i \frac{G_F \varkappa}{\sqrt{2}} \alpha \sqrt{\frac{2}{3}} \rho_0 A_s A_p R_N (1 - 0.41Z^2\alpha^2). \quad (\text{A9})$$

The ratio of Eq. (A9) to Eq. (A5) is

$$\begin{aligned} \frac{\langle s_{1/2} | \mathbf{b} | p_{1/2} \rangle}{\langle s_{1/2} | H_{\text{SI}} | p_{1/2} \rangle} \\ \approx 6 \sqrt{\frac{2}{3}} \frac{\varkappa}{(-Q_W)} (1 - 0.073Z^2\alpha^2). \end{aligned} \quad (\text{A10})$$

3. Scalar-pseudoscalar CP -odd interaction

The Hamiltonian of the scalar-pseudoscalar electron-nucleon (T, P)-odd interaction can be written as [1]

$$H^{\text{SP}} = i \frac{G_F}{\sqrt{2}} A C^{\text{SP}} \gamma_0 \gamma_5 \rho_N(r), \quad (\text{A11})$$

where G_F is the Fermi constant, $A = Z + N$ is the nuclear mass number, Z is the number of protons, and N is the number of neutrons. $C^{\text{SP}} = (ZC_p^{\text{SP}} + NC_n^{\text{SP}})/A$, where C_p^{SP} and C_n^{SP} are the parameters of the scalar-pseudoscalar (T, P)-odd interaction for protons and neutrons, and γ_n are the Dirac matrices.

$$\langle a | H^{\text{SP}} | b \rangle = -\frac{G_F}{\sqrt{2}} \alpha A C^{\text{SP}} \delta_{-\kappa_a, \kappa_b} \int (f_a g_b + g_a f_b) \rho_N dr. \quad (\text{A12})$$

Substitution of the functions (A2) leads to

$$\langle s_{1/2} | H^{\text{SP}} | p_{1/2} \rangle = -\frac{G_F A C^{\text{SP}}}{3\sqrt{2}} \alpha A_s A_p \rho_0 R_N (1 - 0.56Z^2\alpha^2). \quad (\text{A13})$$

Here A_s and A_p are given by Eq. (A3) and ρ_0 is given by Eq. (A6).

4. Electron EDM

The Hamiltonian for the electron EDM interacting with internal atomic electric field \mathbf{E}_{int} can be written as [52]

$$H_e = -d_e (\gamma_0 - 1) \Sigma \cdot \mathbf{E}_{\text{int}}, \quad (\text{A14})$$

where

$$\Sigma = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix},$$

and \mathbf{E}_{int} is the internal atomic electric field. The $s_{1/2}$ - $p_{1/2}$ matrix element can be found in Ref. [53]:

$$\langle s_{1/2} | H_e | p_{1/2} \rangle = -\frac{4Z^3\alpha^2 d_e}{\gamma(4\gamma^2 - 1)(\nu_s \nu_p)^{3/2}}. \quad (\text{A15})$$

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