Parity and time reversal violating nuclear polarizability

V.V. Flambaum, J.S.M. Ginges, and G. Mititelu

School of Physics, University of New South Wales, Sydney 2052, Australia

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Abstract

We propose a nuclear mechanism which can induce an atomic electric dipole moment (EDM). Parity and time reversal violating ($P,T$-odd) nuclear forces generate a mixed $P,T$-odd nuclear polarizability $\beta_{ik}$ (defined by an energy shift $U = -\beta_{ik}E_iH_k$, $E$ is electric field and $H$ magnetic field). The interaction of atomic electrons with $\beta_{ik}$ produces an atomic EDM. We performed an analytical calculation of the $P,T$-odd nuclear polarizability and estimated the value for the induced atomic EDM. The measurements of atomic EDMs can provide information about $P,T$-odd nuclear forces and test models of CP-violation.

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I. CALCULATION OF \( P,T \)-ODD NUCLEAR POLARIZABILITY

Time \((T)\) reversal violation in the interactions of elementary particles has only been indirectly observed in the \( CP \)-violating decay of the neutral K-mesons. The observation of a \( P,T \)-odd multipole (for example, the dominant electric dipole moment (EDM)) of, for instance, an elementary particle or atom would be direct evidence for \( T \)-odd interactions. There are several schemes for incorporating \( CP \)-violation into unifying theories. These schemes make very different predictions for the value of EDMs of particles and atoms. While there has never been an unambiguous detection of these EDMs, upper limits on their values provide stringent tests of competing models of \( CP \)-violation.

In this paper we propose a mechanism which can induce an atomic EDM: the interaction of a \( P,T \)-odd perturbed nucleus with the electric and magnetic fields of an external electron.

The interaction of external electric \( E \) and magnetic \( H \) fields with operators of nuclear electric and magnetic dipole moments, \( d \) and \( \mu \), gives rise to an energy shift,

\[
U = -\beta_{ik}E_iH_k,
\]

where \( \beta_{ik} \) is the mixed \( P,T \)-odd nuclear polarizability [1]. Parity and time reversal violating \((P,T\)-odd\) nuclear forces generate this polarizability,

\[
\beta_{ik} = 2\sum_n \frac{\langle \tilde{\psi}_0|d_i|\tilde{\psi}_n\rangle\langle \tilde{\psi}_n|\mu_k|\tilde{\psi}_0\rangle}{E_n - E_0},
\]

(1)

where \( \tilde{\psi}_0 \) and \( \tilde{\psi}_n \) are \( P,T \)-odd perturbed ground and excited nuclear states, respectively. We consider a heavy spherical nucleus with a single unpaired nucleon. The \( P,T \)-odd interaction between the non-relativistic nucleon and the nuclear core is given by (see, e.g. [2])

\[
\hat{H}_{PT} = \frac{G}{\sqrt{2}m} \eta \sigma \nabla \rho(r),
\]

(2)

\( G \) is the Fermi weak interaction constant, \( \eta \) is a constant which characterizes the strength of the \( P,T \)-odd nucleon-nucleon interaction (limits on \( \eta \) have been obtained from atomic [3] and molecular [4] experiments), \( \sigma \) is the nuclear spin operator, \( \rho(r) \) is the density of the nuclear core, and \( m \) is the proton mass. The \( P,T \)-odd perturbed nuclear wavefunctions resulting from the interaction \( \hat{H}_{PT} \), in an approximation where the nuclear density \( \rho \) and potential \( U \) coincide, \( \rho_0(r) = U(r)\rho_0(0)/U(0) \), have the form [4]

\[
\tilde{\psi}_n = (1 - \xi \sigma \cdot \nabla)\psi_n,
\]

(3)

where \( \xi = -\eta \frac{G \rho_0(0)}{2\sqrt{2m}U(0)} \) and \( \psi_n \) is an unperturbed wavefunction.

In lowest order in the \( P,T \)-odd interaction the polarizability (Eq. [1]) is

\[
\beta_{ik} = \sum_n \frac{2\xi}{E_n - E_0} \left\{ \langle \psi_0|[(\sigma \cdot \nabla),d_i]|\psi_n\rangle\langle \psi_n|\mu_k|\psi_0\rangle + \langle \psi_0|d_i|\psi_n\rangle\langle \psi_n|[(\sigma \cdot \nabla),\mu_k]|\psi_0\rangle \right\}
\]

(4)

\[
= \beta_{ik}^{(1)} + \beta_{ik}^{(2)}.
\]

(5)

In the non-relativistic approximation, the only contribution to the first term of this equation arises due to transitions between fine-structure doublets, for example \( p_{1/2} \) and \( p_{3/2} \), \( d_{3/2} \) and \( d_{5/2} \) (because the only non-zero matrix elements of \( \mu \) are between these states). In the second term, states \( \psi_n \) must have opposite parity to \( \psi_0 \) (because the matrix element of...
\(d = er\) cannot mix states of the same parity. The largest contributions to this term arise due to transitions to the next shell. Therefore the energy denominator of the second term is much larger than that of the first.

The nuclear electric dipole operator is defined as \(d = e_N r\), where \(e_N\) is the effective charge for the nucleon \(N = n, p\), \(e_p = (N/A)e\), \(e_n = -(Z/A)e\), which appears due to the recoil effect. The nuclear magnetic dipole operator is defined as \(\mu = \mu_N (g_l + g_s s)\), where \(\mu_N\) is the nuclear magneton, \(g_s\) and \(g_l\) are the spin and orbital \(g\)-factors; for the proton \(g_s = 5.586, g_l = 1\) while for the neutron \(g_s = -3.826, g_l = 0\).

The first term of Eq. (4) can be expressed as

\[
\beta_{ik}^{(1)} = e_N \mu_N \xi (g_s - g_l) \frac{1}{\omega_{Fs}} \langle \psi_0 | \sigma_i | \psi_{i'} \rangle \langle \psi_{i'} | \sigma_k | \psi_0 \rangle,
\]

where \(\omega_{Fs} = E_{i'} - E_0\) is the energy difference between the fine structure components \(\psi_0\) and \(\psi_{i'}\).

Let us now consider the second term of Eq. (4), \(\beta_{ik}^{(2)}\). This can be written as

\[
\beta_{ik}^{(2)} = \sum_n \frac{\xi \mu_N}{E_n - E_0} \left\{ g_s \langle \psi_0 | d_i | \psi_n \rangle \langle \psi_n | [\sigma_j, \sigma_k] \nabla_j | \psi_0 \rangle + 2g_l \langle \psi_0 | d_i | \psi_n \rangle \langle \psi_n | \sigma_j [\nabla_j, l_k] | \psi_0 \rangle \right\}.
\]

Using the commutation relations \([\sigma_j, \sigma_k] = 2i \epsilon_{jkm} \sigma_m\) and \([\nabla_j, l_k] = i \epsilon_{jkm} \nabla_m\), we obtain

\[
\beta_{ik}^{(2)} = 2i \xi \mu_N (g_s - g_l) \epsilon_{jkm} \sum_n \frac{\langle \psi_0 | d_i | \psi_n \rangle \langle \psi_n | \sigma_j \nabla_m | \psi_0 \rangle}{E_n - E_0}.
\]

This term can be further simplified by replacing the operator \(\nabla\) by the commutation relation \(\nabla = m[H, \hat{r}]\), where \(\hat{H} = \hat{p}^2/2m + \hat{V}(r)\) is the single-particle Hamiltonian. Neglecting the spin-orbit interaction, that is setting \([\hat{H}, \sigma] = 0\), and using closure, \(\sum_n | \psi_n \rangle \langle \psi_n | = 1\), Eq. (8) becomes

\[
\beta_{ik}^{(2)} = -2i \xi \epsilon_N \mu_N m (g_s - g_l) \epsilon_{kjm} \langle \psi_0 | r_i \sigma_j r_m | \psi_0 \rangle.
\]

So, to first order in the \(P, T\)-odd interaction, we can write the nuclear polarizability as

\[
\beta_{ik} = \epsilon_N \mu_N (g_s - g_l) \{ (1/\omega_{Fs}) \langle \psi_0 | \sigma_i | \psi_{i'} \rangle \langle \psi_{i'} | \sigma_k | \psi_0 \rangle - i2m \langle \psi_0 | r_i (\sigma \times r_m) | \psi_0 \rangle \}.
\]

The \(P, T\)-odd nuclear polarizability can be expressed in terms of scalar and tensor components,

\[
\beta_{ik} = \delta_{ik} \beta_s + [I_i I_k + I_k I_i - \frac{2}{3} \delta_{ik} I(I+1)] \beta_t,
\]

\(I\) is the nuclear total angular momentum. We are interested in finding the scalar and tensor \(P, T\)-odd polarizabilities, \(\beta_s\) and \(\beta_t\). Let us start with the scalar contribution. Now, from Eq. (11) we see that \(\beta_s = \beta_{ii}/3\). We can see from Eq. (10) that there is no scalar contribution from the second term, since \(r_i (\sigma \times r)_i = 0\). We can therefore write the scalar term as

\[
\beta_s = \xi \epsilon_N \mu_N (g_s - g_l) \left( \frac{1}{3 \omega_{Fs}} \right) \langle \psi_0 | \sigma_i | \psi_{i'} \rangle \langle \psi_{i'} | \sigma_i | \psi_0 \rangle.
\]
Evaluating this expression using spherical spinors, with the ground state wavefunction \( \psi_0 \) corresponding to \( I = l + 1/2 \) and its fine-structure partner \( \psi_{0'} \) corresponding to \( I' = l - 1/2 \), \( l \) is the orbital angular momentum, we obtain

\[
\beta_s = \xi e_N \mu_N (g_s - g_l) \left( \frac{1}{\omega_{fs}} \right) \left( \frac{2I - 1}{3I} \right). \tag{13}
\]

Let us now consider the tensor polarizability \( \beta_t \). Setting \( i, k = z \) in Eq. (10) and taking the maximum projection, \( I_z = I = l + 1/2 \), the first term is zero, since \( \psi_{0'} \) with maximum projection \( I_{z}' = I' = l - 1/2 \) gives zero contribution. The second term is also zero in this case, since \( \sigma_x \) and \( \sigma_y \) cannot have diagonal matrix elements. Using Eq. (11) with \( \beta_{zz} = 0 \) we obtain

\[
\beta_t = -\frac{3\beta_s}{2I(2I - 1)}. \tag{14}
\]

Inserting Eqs. (13) and (14) into Eq. (11), we obtain for the nuclear \( P,T \)-odd polarizability

\[
\beta_{ik} = \xi e_N \mu_N (g_s - g_l) \left( \frac{1}{\omega_{fs}} \right) \left( \frac{2I - 1}{3} \right) \frac{1}{I} \delta_{ik} - \frac{1}{2I} [I_i I_k + I_k I_i - \frac{2}{3} \delta_{ik} I(I + 1)]. \tag{15}
\]

Note that in spherical nuclei the tensor part arises due to unpaired nucleons only. The scalar part does not require nuclear spin, therefore several nucleons can contribute to it; however, if all states in a fine-structure doublet are occupied, then the contributions cancel exactly.

It is interesting to consider the \( P,T \)-odd nuclear polarizability of a deformed nucleus. In this case we would expect contributions to the EDM from many nuclei (collective polarizability) because in deformed nuclei about \( A^{2/3} \) nucleons are in open shells. This enhancement is similar to that of the \( P,T \)-odd nuclear quadrupole moment discussed in [5].

II. ESTIMATE FOR INDUCED ATOMIC EDM

Consider an atom with one external electron above closed shells. We are interested in the atomic EDM induced by the interaction of atomic electrons with the \( P,T \)-odd perturbed atomic nucleus polarized by the fields of the external electron (we use the nuclear model defined in the previous section). The induced atomic EDM arises in the third order of perturbation theory,

\[
d_{\text{atom}} = \sum_{n,n',m,m'} \langle 0, 0'| d_z | n', n \rangle \langle n, n'| \hat{H}_E | m', m \rangle \langle m, m'| \hat{H}_B | 0', 0 \rangle (E_0 + E_{0'} - E_n - E_{n'}) (E_0 + E_{0'} - E_m - E_{m'}) + \text{permutations}, \tag{16}
\]

where unprimed states \((m, n, 0)\) denote electronic states, primed states \((m', n', 0')\) denote \((P,T\)-odd perturbed\) nuclear states, and the electric and magnetic interactions between the external electron and the unpaired nucleon are

\[
\hat{H}_E = -\frac{e}{R^3} d_n \cdot \mathbf{R}, \quad \hat{H}_B = -\frac{e}{R^3} \mu_n \cdot (\mathbf{R} \times \alpha), \tag{17}
\]

\( d_n \) and \( \mu_n \) are the electric and magnetic dipole moments of the nucleus, and \( \alpha \) is the electron Dirac matrix. We use the Dirac interaction because the external electron close to the nucleus is relativistic.
To measure an EDM, an external electric field is applied to the system which couples to the electron electric dipole moment operator $d_z$. Terms in which this operator admixes excited states, for example

$$
\sum_{m,n,n'} \langle 0, 0'| \hat{H}_E | n', n \rangle \langle n, n'| d_z | n', m \rangle \langle m, n'| \hat{H}_B | 0', 0 \rangle
$$

have very large (nuclear) energy denominators as here the electric field interacts with the excited states of the atom. We can therefore neglect this contribution to the atomic EDM.

The atomic EDM induced by the interactions (Eq. 17) can therefore be presented as

$$
d_{\text{atom}} \approx 2 \sum_n \langle 0 | d_z | n \rangle \langle n | \hat{H}_E | 0 \rangle \equiv 2 \sum_n \langle 0 | d_z | n \rangle \langle n | \hat{H}_{P,T} | 0 \rangle,
$$

(19)

where we have set $n' = 0'$, because $d_z$ does not act on the nuclear wavefunctions. Typical electron energies are much smaller than nuclear energies, $(E_0 - E_m) << (E_0' - E_{m'})$, therefore we have used closure for the electron states, $\sum_m |m\rangle \langle m| = 1$. Substituting Eq. (17) into Eq. (19), and using the definition for the $P,T$-odd nuclear polarizability (Eq. (1)), we obtain

$$
d_{\text{atom}} \approx 2 e^2 R^6 \epsilon_{ikp} \beta_s \sum_n \langle 0 | d_z | n \rangle \langle n | R_i R_k \alpha_p | 0 \rangle \frac{E_0 - E_n}{E_0 - E_n}
$$

(20)

where we have defined an effective Hamiltonian $\hat{H}_{P,T}$ which describes the interaction of the $P,T$-odd nuclear polarizability with atomic electrons.

In this approximation, the contribution of the scalar polarizability to the atomic EDM is zero ($R \cdot [R \times \alpha] = 0$). However, there is no theorem which forbids this contribution. Indeed, consider non-relativistic expressions for magnetic and electric fields produced by a charged particle with magnetic moment $\mu = \mu_s$,

$$
\mathbf{H} = e \frac{\mathbf{n} \times \mathbf{v}}{R^2} + \frac{3(\mathbf{n} \cdot \mathbf{\mu}) \mathbf{n} - \mathbf{\mu}}{R^3} + \frac{8\pi}{3} \mu\delta(R) \\
\mathbf{E} = e \frac{\mathbf{n}}{R^2},
$$

(21)

where $\mathbf{v}$ is the velocity of the particle, $\mathbf{n} = \mathbf{R}/R$. Substituting these expressions into the interaction energy

$$
\beta_s \delta_{ik} H_i E_k = 2e\mu \beta_s \frac{\mathbf{s} \cdot \mathbf{n}}{R^2} \left( \frac{1}{R^3} + \frac{4\pi}{3} \delta(R) \right),
$$

(22)

we see that the first, longer-range orbital field in the expression for $\mathbf{H}$ indeed does not give any contribution to the interaction. However, the spin magnetic field, which decays more rapidly with distance, does contribute. The angular structure of the effective interaction (Eq. 22) is similar to that between an electron EDM and an atomic electric field (see, e.g., [6]). However, the interaction (Eq. 22) decays with distance very rapidly, and is very singular at small distances. This strong singularity is an indication that one should use the relativistic form for the magnetic interaction (Eq. [17]) in order to describe the small distance contribution correctly. We showed above that in this case our calculation gives zero for the $\beta_s$ contribution to the EDM.
The only contribution of the nuclear $P,T$-odd polarizability to the atomic EDM therefore arises due to the tensor term. Inserting the expression for $\beta_{ik}$ (Eq. 15) into the above expression (Eq. 20) we obtain for the effective Hamiltonian $\hat{H}_{PT}$

$$\hat{H}_{PT} = -\frac{e^2}{2R^6}e_N\xi_N(g_s - g_l)(\frac{1}{\omega_{Is}})^2\epsilon_{klp}R_iR_l\alpha_p[I_iI_k + I_kI_i - \frac{2}{3}\delta_{ik}I(I + 1)].$$

(23)

In earlier works the value of atomic EDMs of Cs $[7,2]$, Dy $[8,5]$ and Ra $[9,10]$ induced by the $(P,T$-odd) nuclear magnetic quadrupole moment (MQM) have been calculated. It is therefore useful to compare $\hat{H}_{PT}$ with the Hamiltonian $\hat{H}_{MQM}$ which describes the interaction of a nuclear MQM with atomic electrons,

$$\hat{H}_{MQM} = \frac{Me}{R^5 2I(2I - 1)}\epsilon_{klp}R_iR_l\alpha_p\{I_iI_k + I_kI_i - \frac{2}{3}\delta_{ik}I(I + 1)\},$$

(24)

so as to obtain an estimate for the value of the atomic EDM induced by the nuclear polarizability. Here $M$ is the magnetic quadrupole moment which, for $I = I + 1/2$, is $M = -\xi_N(g_s - 2g_l)(2I - 1)$. The ratio of $\hat{H}_{PT}$ to $\hat{H}_{MQM}$ is

$$\frac{\hat{H}_{PT}}{\hat{H}_{MQM}} = \frac{1}{R}(g_s - 2g_l)\omega_{Is}.$$  

(25)

The largest contribution to the atomic EDM arises due to mixing between $s$ and $p_{3/2}$ electron states. The radial integral for the magnetic quadrupole converges at $R \sim a_B/Z$ $[2]$, where $a_B$ is the Bohr radius. The $\hat{H}_{PT}$ matrix element is more singular at the nucleus than that of $\hat{H}_{MQM}$. Considering $s$ and $p_{3/2}$ mixing, the EDM induced by the nuclear polarizability contains an extra factor

$$S_{rel} \equiv -\gamma_1 + \gamma_2 - 2\frac{a_B}{Z}\frac{R_N}{(2I - 1)^3},$$

(26)

where $R_N$ is the nuclear radius, $\gamma_1 = \sqrt{1 - Z^2\alpha^2}$ and $\gamma_2 = \sqrt{4 - Z^2\alpha^2}$. For $Z^2\alpha^2 << 1$,

$$S_{rel} \approx \frac{4}{3}\frac{1}{Z^2\alpha^2}\frac{R_N}{a_B}.$$

(27)

has a very weak dependence on the nuclear radius $R_N$ which we use as a cut-off parameter in the integration over $R$. Therefore, the ratio of $\hat{H}_{PT}$ to $\hat{H}_{MQM}$ is

$$\frac{\hat{H}_{PT}}{\hat{H}_{MQM}} \sim \frac{Ze^2 S_{rel}}{a_B\omega_{Is}}.$$  

(28)

For heavy atoms this ratio is of the order of 1%.

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