New bounds on the electric dipole moment of the electron and on T-odd electron-nucleon coupling

V. V. Flambaum and I. B. Khriplovich
Institute of Nuclear Physics, Siberian Division, Academy of Sciences of the USSR

The electric dipole moment (EDM) of the electron, together with the hyperfine coupling, induces an EDM in atoms and molecules with closed electron shells. Experiments with $^{129}$Xe and TIF have yielded bounds on the EDM of the electron ($d/e |e|$ = $(0.4 \pm 1.4) \cdot 10^{-26}$ cm) and on the T-odd scalar electron-nucleon coupling constant.

A recent experiment\(^1\) yielded a very stringent bound on the electric dipole moment (EDM) of the $^{129}$Xe atom:

$$d^{(129}\text{Xe}) = (-0.3 \pm 1.1) \cdot 10^{-26} |e| \text{cm.} \quad (1)$$

This in turn leads to bounds on the electron-nucleon\(^2\) and nucleon-nucleon\(^3\) T-odd coupling constants and on the EDM of the proton\(^4\). It was noted in Ref. 6 that because of the hyperfine (HF) interaction the electron EDM can also induce a dipole moment in atoms and molecules with closed electron shells, in particular in the xenon atom and the TIF molecule. However, to date, only the ground state $^1S_0$ is known to be the only closed shell for xenon.

It is convenient to begin by considering a mechanism that gives rise to the EDM of the electron, not connected directly to the hyperfine interaction—a direct coupling of the EDM of the electron to the magnetic field of the magnetic moment of the nucleus. The interaction of the EDM of an electron $d$ with a tensor electromagnetic field $F_{\mu\nu}$ is described by the following relativistically invariant form:

$$\mathcal{H} = \frac{d}{2} \bar{\psi} \gamma_\mu d \gamma^\mu F_{\mu\nu}.$$ \quad (2)

Here

$$\bar{\psi} = \left( \begin{array}{c} \psi_3 \ni \end{array} \right), \quad \gamma_\mu = \left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right)$$

$$\bar{\psi} = \bar{\psi} \gamma_1 \gamma_\sigma \gamma_\rho \gamma_\tau,$$ and $\sigma$ and $\gamma$ are radial wave functions, $\Omega_\sigma$ is a spherical spinor, $j = 1$ and $l, l', m$ are the total and orbital moments of the electron, $l = 2j - 1, m_{\sigma} = 1/2 \gamma_\sigma (\gamma_{\rho}, \gamma_{\tau})$, and the $\gamma_\sigma$ are Dirac matrices. We now easily find that the interaction of the EDM with the magnetic field has the form:

$$\mathcal{H} = -i d \bar{\psi} \gamma_\tau H,$$ \quad (3)

where $H$ is the magnetic field of the nucleus with magnetic moment $\mathcal{M}$:

$$H = -g \left[ \frac{\mathcal{M}}{r} \right] = \frac{3(\mathcal{M}r \mathcal{M}r' - \mathcal{M}r' \mathcal{M}r)}{r^2} - \frac{8\chi}{3} \mathcal{M}(r).$$ \quad (4)

The expression for $d_\tau$, the atomic EDM induced by the

$$d_\tau = \sum_{\sigma} \frac{1}{2} (-1)^{\sigma_3} \left( 0 | n_{\sigma} \left| n_{\sigma} \right) \langle n_{\sigma} | V | n_{\sigma} \right) / (E_{\text{tot}} - E_n). \quad (5)$$

A naive evaluation of the expression (5) would give $d_\tau \sim Z^2 \alpha^2 (m/M)$. The simplest way to see this is to look at the contribution from the last term in (4): $\langle n_{\sigma} | V | n_{\sigma} \rangle \sim (\gamma - Z/a)$, where $a$ is the Bohr radius. However, we take account of the fact that in the nonrelativistic limit the operator (3) is proportional to the spin:

$$V = -\frac{2m}{2\alpha} \mathbf{s} \sigma (\mathbf{p} l \mathcal{M} - \mathbf{H}).$$ \quad (6)

Such a computation is given here. It is of interest, in our opinion, also from the viewpoint of atomic theory. The method of calculation that we use has allowed us to find the EDM of an atom subject to a T-odd scalar electron-nucleon interaction. Moreover, we have estimated the correction, due to the HF interaction, that is to be applied to the T-invariant effects of nonconservation of spatial parity in atoms, as a function of the spin of the nucleus.

This in turn leads to bounds on the EDM of the proton\(^3\). It was noted in Ref. 6 that because of the hyperfine (HF) interaction the electron EDM can also induce a dipole moment in atoms and molecules with closed electron shells, in particular in the xenon atom and the TIF molecule. However, up to now no real computation of this effect has been made.

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In the real situation, where $R \leq 1$, the accuracy is of order $Z^2a^2$. The singular matrix element in the operator $V$ is

$$\langle n_1 | V | p_\mu \rangle = \delta (|y|) \frac{Z^2}{3} \sum_{\nu, \lambda} \left\{ \frac{6}{\rho} + \frac{6}{\rho^2} \right\} \delta (\rho) \langle \lambda | \hat{S}_\mu \hat{S}_\nu \rangle.$$  \hspace{1cm} (10)

Using the identity

$$\frac{d}{dr} (p_\mu p_\nu) = \frac{2}{\rho} \hat{S}_\mu \hat{S}_\nu,$$  \hspace{1cm} (11)

which follows from the radial Dirac equation at small distances, we can express the matrix element (10) via the matrix element of the operator $y_\mu (r)$.

The identity (12) holds to within a correction term $-Z^2a^2/4$. We note that to this precision the result does not depend on the specific method of computing the finite dimensions of the nucleus (cf. the calculation of the weak interaction in atoms).

The EDM of the xenon atom, subject to the $T$-odd interaction of the electron with the nucleons, was calculated. By comparing the formulae (12) and (14) we infer that the EDM of xenon, as induced by the interaction $V$, may be derived from the results of the contact model without further calculation. We now need only to take into account the contribution from $p_{\text{3d}}$-electrons, reducing to the substitution $R \rightarrow R - 1$; in the case (14) of pure contact interaction the contribution from the $p_{\text{3d}}$-electrons is absent.

We must employ this strategy of keeping terms that are singular in $r_\nu$, also in calculating the EDM of atoms when we treat simultaneously the hyperfine interaction

$$U = |e| \langle n_1 | M | n_0 \rangle$$  \hspace{1cm} (15)

and the $T$-odd interaction of the EDM of the electron with the nuclear field (cf. (2)): 

$$W = -d_0 [x] = \frac{Z e}{\rho} \gamma_\mu n_0.$$  \hspace{1cm} (16)

Here

$$\alpha = \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix}, \quad \sum_{\lambda} \begin{pmatrix} \sigma \lambda & 0 \\ 0 & \sigma \lambda \end{pmatrix}, \quad n = \frac{r}{r}.$$  \hspace{1cm} (17)

The EDM of the atom induced by this interaction arises in third-order perturbation theory

$$d_0 = \sum \langle n_1 | x | n_0 \rangle \langle U | k | k \rangle \langle k | W | x \rangle \langle x | U | n_1 \rangle,$$  \hspace{1cm} (18)

where the ellipsis stands for the set of permuted terms. We note immediately that the effect

$$d_0' = \sum \langle n_1 | d_0 \gamma_\mu | n_0 \rangle \langle U | k | k \rangle \langle k | W | x \rangle \langle x | U | n_1 \rangle$$  \hspace{1cm} (19)

arising in the second-order approximation has the order of magnitude $d_0' \sim -Z^2a^2/(m_e/r_\nu)$ and may be neglected compared to (8).

The matrix elements of the operators $U$ and $V$ are not in themselves singular with respect to $r_\nu$. One may suspect, however, that an $r_\nu$-singularity arises in sums of the form

$$\sum \langle n_1 | U | k \rangle \langle k | W | x \rangle \langle x | U | n_0 \rangle$$  \hspace{1cm} (20)

because of the contributions from high energy intermediate states $|k\rangle$.

We therefore consider the correction

$$\langle 0 | \langle n_1 | U | k \rangle \langle k | W | x \rangle \langle x | U | n_0 \rangle | 0 \rangle$$  \hspace{1cm} (21)

to the wave function $|0\rangle$ in the region $r \geq r_\nu$. Applying the operator $H - E_n$ and making use of the completeness condition, we easily arrive at the Dirac radial equations for this correction:

$$f' + \frac{1}{r} - \frac{Z e}{r} \gamma_\mu f = \frac{1}{\rho} Z e d \gamma_\mu d^{-1},$$  \hspace{1cm} (22)

$$g' + \frac{1}{r} + \frac{Z e}{r} \gamma_\mu g = \frac{1}{\rho} Z e d \gamma_\mu d^{-1}.$$  \hspace{1cm} (23)

Here we have omitted the mass and energy of the electron, which are negligible for $r \geq r_\nu$, and we have also assumed that the orbital moment of the correction $|0\rangle$ is $1 = 2j - 1$. The driven solution of (20) has the form:

$$\langle 0 | \langle n_1 | U | k \rangle \langle k | W | x \rangle \langle x | U | n_0 \rangle | 0 \rangle = \frac{Z e}{2} d \gamma_\mu d^{-1}.$$  \hspace{1cm} (24)

The homogeneous solution $r^{-1}$ is less singular as $r \rightarrow 0$ and at small distances is negligible. A singular homogeneous solution $r^{-1}$ appears as consequence of an accurate formulation of the boundary conditions on the nucleus. However, it is significant only in the immediate neighborhood of the nucleus, and its relative contribution to the matrix element $\langle n_1 | U | 0 \rangle$ is on the order of $Z^2a^2/2$.

It is convenient to introduce the effective operator

$$W' = \sum \langle \kappa | x | \kappa \rangle \langle \kappa | W | \kappa \rangle \langle \kappa | U | n_1 \rangle.$$  \hspace{1cm} (25)

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By making use of (15), (22), and (21) we see that as \( r \to 0 \) we have \( W = U/r = 1/r^\alpha \) and the matrix element \( \langle \alpha | W | \beta \rangle \) diverges as \( r \to 0 \). Using (22) we find, after some simple but rather lengthy transformations,

\[
\langle \alpha | W | p_\beta \rangle \approx \frac{2\alpha}{3} \frac{4}{3} \frac{1}{2} \frac{M}{M} k \Theta (0, r^\alpha) \langle p_\beta | \rangle.
\]  

We can derive this result in another way, using the equations for the correction to the wave function that arises from the hyperfine interaction. Here the solutions have the form

\[
\langle \alpha | W | p_\beta \rangle = \left( \begin{array}{c} \alpha \Theta_k \langle p_\beta | \rangle \\
(\alpha + 1) \Theta_k \langle p_\beta | \rangle \\
(\alpha + 2) \Theta_k \langle p_\beta | \rangle \\
\end{array} \right).
\]

We note that the terms in (17) containing the matrix elements \( \langle \alpha | p_\beta \rangle \) between the intermediate states \( |\alpha \rangle \) and \( |\beta \rangle \) are negligible since these terms have no singularities with respect to \( r_0 \).

By comparing (24) and (12) we see that the contribution \( W \) dominates. The final value of the matrix element of the mixture is

\[
\langle \alpha | W | p_\beta \rangle = \frac{2\alpha}{3} \frac{4}{3} \frac{1}{2} \frac{M}{M} p \langle \alpha | p_\beta \rangle.
\]  

We now note that (17) and (20) both vanish in the nonrelativistic limit for closed electron shells. The sum of the \( W \) operators over all the electrons is proportional to their total spin, which is zero in the ground state \( |0\rangle \) and in the states \( |\beta \rangle \). Thus we again find that the contributions of the \( p_\beta \) and \( p_\alpha \) electrons cancel. We reflect this by substituting \( R = R - 1 \) in the final solution.

The numerical calculations\(^7\) (cf. also [2]) yields the following expression for the EDM of xenon via the coupling constants (14):

\[
d(n = 0) = 0.41 \times 10^{-7}|e| e\Sigma.
\]  

By comparing the matrix elements (26) and (14) and the result (27) we infer that

\[
d(n = 3) = -1.3 \times 10^{-7}|e| e\Sigma = -0.8 \times 10^{-7}|e| e.
\]  

Using the experimental result (1) we find the following bound on the EDM of the electron

\[
d(\alpha = 0) = (0.4 \pm 1.4) \times 10^{-7}|e| e\Sigma.
\]  

The theoretical error in this result arises from the inexact calculation of the terms \( Z^2 \alpha^2 \) and from the error in the Hartree-Fock calculations in Ref. 3 which gave rise to the expression (27). Thus the total error in our calculations does not appear to exceed 30-40%.

The bound (28) is several times weaker than the better one derived from experiments on cesium and xenon atoms in the metastable \( P_2 \) state.\(^8\) We note, however, that the authors of Ref. 1 intend to increase the accuracy of their results to fourth order.

Ref. 1 discusses the possibility of measuring the EDM of mercury, where the effect of \( T \)-invariance is remarkably large. Using the proportionality of the matrix elements (26) and (14) and the calculations with the Hamiltonian (14) in Ref. 2 we find

\[
d(3P_{1/2}) = -1.4 \times 10^{-7}|e| e.
\]  

With the aid of the \( V \) and \( \bar{V} \) operators we are led from the EDM of the electron to the \( P \) and \( T \)-odd dipole moments of polar molecules in stationary states with paired electrons. Using the bounds on the constants in the Hamiltonian (14) as derived from experiments with the TIF molecule\(^9\) we find via (26) that

\[
d = (0.9 \pm 1.3) \times 10^{-11}|e| e\Sigma.
\]

This bound is fully comparable with (29), but the precision of the molecular estimate is better than the atomic.

Because of the hyperfine interaction, an EDM is also induced in atoms and molecules with closed electron shells by \( T \)-odd interactions between the electron and the nucleus:\n
\[
\frac{\mu}{N} \sum_{i=1}^{n} \frac{k_i N_i}{N}.
\]

In this case the Hamiltonian of the electron-nucleus interaction is, in the limit for an infinitely heavy nucleus,

\[
H = n \alpha \eta \sum_{i=1}^{n} \frac{k_i N_i}{N}.
\]

Here \( \eta \) is the atomic number. The EDM of the atom arises in the third-order perturbation theory with only the need to replace \( W \) by \( H \), in a formula of the type of (17). Using (25) for the correction to the wave function due to the \( H \) interaction we find the effective matrix element of the mixture

\[
\langle \alpha | H | p_\beta \rangle = 2 \frac{\alpha}{n} \sum_{i=1}^{n} \langle \alpha | p_\beta \rangle.
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\]
we may neglect the HF interaction. In the lowest nonvanishing approximation with respect to $m^{-1}$ the corresponding Hamiltonian of the electron-nucleus interaction reduces to the form

$$H_{t} = \frac{G}{\sqrt{2}} \sum_{x} \left( h_{\mu} \sum_{x} \psi_{\mu}(x) \right) \mathbf{\sigma} \cdot \mathbf{\mathbf{\sigma}}_{x},$$

(36)

The matrix element of the mixture is

$$\langle \psi_{\mu} | H_{t} | \psi_{\mu} \rangle = 2 \sqrt{2} \sum_{x} \langle \psi_{\mu} | \psi_{\mu}(x) \rangle \mathbf{\sigma} \cdot \mathbf{\mathbf{\sigma}}_{x}.$$

(37)

The cesium experiment yields

$$k_{e} = (-0.3 \pm 1.1) \cdot 10^{-3},$$

(38)

and the TIF experiment yields

$$k_{e} = (2.5 \pm 3.8) \cdot 10^{-3}.$$  

(39)

The bounds on the constants $k_{e}$ and $k_{en}$ that are derived from other experiments are far weaker than (38) and (39).

We note in conclusion that the HF interaction also leads to the nuclear spin dependence of the matrix element in the $T$-invariant interaction of the vector electron and axial nucleon neutral currents. The corresponding effective operator (cf. (23), (24), and (33)) is

$$B = \frac{G}{\sqrt{2}} \sum_{x} \rho_{x},$$

$$g = \frac{1}{2} Q_{W} \frac{g_{\mu}}{m_{e}} = -2.5 \cdot 10^{-3} A \mu_{N}.$$  

(40)

Here $I$ is the spin of the nucleus, $Q_{W} = 0.55$, and $A$ is the weak charge of the nucleus. The dimensionless constant $g$ is comparable in magnitude with the corresponding constant characterizing the coupling of the vector electron and axial nucleon neutral currents. It is less by roughly an order of magnitude that the contribution from the anapole moment of the nucleus, at least, in the case of non-paired protons.19

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