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

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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 TlF have yielded bounds on the EDM of the electron ($d/|e| = (0.4 \pm 1.4) \cdot 10^{-23}$ cm; $(0.9 \pm 1.3) \cdot 10^{-23}$ 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:

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

This in turn leads to bounds on the electron-nucleon[2,3] and nucleon-nucleon[3–5] *T*-odd coupling constants and 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 TlF molecule. However, up to now no real computation of this effect has been made.

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.

It is convenient to begin by considering a mechanism that gives rise to the EDM of the atom, 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 $F_{\mu\nu}$ we write in the following relativistically invariant form:

$$H_d = \frac{d}{2} \bar{\psi} \gamma_5 \sigma_{\mu\nu} \psi F_{\mu\nu}. \tag{2}$$

Here

$$\psi = \begin{pmatrix} f\Omega_{jl} \\ ig\Omega_{j\bar{l}} \end{pmatrix}, \quad \gamma_5 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

$\bar{\Psi} = \Psi^+\gamma_0$, f and g are radial wave functions, Ω_{jl} is a spherical spinor, j and l are the total and orbital moments of the electron, $\bar{l} = 2j - l$, $\sigma_{\mu\nu} = 1/2(\gamma_\mu \gamma_\nu - \gamma_0\gamma_\mu)$, and the γ_μ are Dirac matrices. We now easily find that the interaction of the EDM with the magnetic field has the form:

$$V = -id\boldsymbol{\gamma}\mathbf{H}, \tag{3}$$

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

$$\mathbf{H} = \left[\nabla\left[\nabla\frac{1}{r}, \mathbf{M}\right]\right] = \frac{3(\mathbf{Mr})\mathbf{r} - \mathbf{M}r^2}{r^5} - \frac{8\pi}{3}\mathbf{M}\delta(\mathbf{r}). \tag{4}$$

The expression for d_V, the atomic EDM induced by the interaction (3), has the form

$$\mathbf{d}_V = \sum_n \frac{\langle 0|V|n\rangle\langle n|e\mathbf{r}|0\rangle + \langle 0|e\mathbf{r}|n\rangle\langle n|V|0\rangle}{E_0 - E_n}. \tag{5}$$

A naive evaluation of the expression (5) would give $d_V \sim Z^2\alpha^2(m/m_p)d$. The simplest way to see this is to look at the contribution from the last term in (4): $\Psi^2(0) \sim Z/a^3$, $\langle\gamma\rangle \sim Z\alpha$, 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:

$$V = -\frac{d}{2m}\boldsymbol{\sigma}([\mathbf{pH}] - [\mathbf{Hp}]). \tag{6}$$

Since the matrix element $\mathbf{r}$ does not act on the spin variables, the total spin vanishes for atoms with complete shells, not only in the ground state $|0\rangle$ but also in intermediate states $|n\rangle$. Therefore in this limit the expression (5) reduces to 0. More precisely, when we sum over complete shells an additional small quantity $\sim Z^2\alpha^2$ must appear in the expression for d_V.

In fact, even for relatively small values of $Z^2\alpha^2$ the situation turns out to be much more favorable. The reason is that in a relativistic treatment the matrix element $\langle s_{1/2}|V|p_{1/2}\rangle$ becomes infinite in the limit of a point nucleus. In the case of a finite radius r_0 for the nucleus this matrix element contains a relativistic amplification factor

$$R = \left(\frac{a}{2Zr_0}\right)^{2-2\gamma} \frac{4}{[\Gamma(2\gamma+1)]^2}, \quad \gamma = (1 - Z^2\alpha^2)^{1/2}, \tag{7}$$

which tends to 1 as $Z^2\alpha^2 \to 0$, but even for $Z^2\alpha^2 = 0.16$ (we have Xenon in mind) is significantly different from 1, $R(\mathrm{Xe}) = 2.7$. This amplification factor, which is singular as a function of r_0, is missing from the remaining matrix elements. Therefore the compensation for the contributions from the closed $p_{1/2}$ and $p_{3/2}$ subshells leads to the appearance of a multiplier R-1 in the expression for d_V, which the case of xenon is by no means numerically small, even though it vanishes as $Z^2\alpha^2 \to 0$:

$$d_V \sim (R-1) Z^2\alpha^2 (m/m_p) d. \tag{8}$$

From now on we shall take account of only the term which is singular in r_0 in the expression for the dipole moment of the atom. The expression R-1 corresponds to the summation of the leading terms in $\ln(a/2Zr_0)$ in the perturbation expansion for a small parameter $Z^2\alpha^2$. Therefore the accuracy of such a computation as $Z^2\alpha^2 \to 0$ is

$$Z^2\alpha^2/(R-1) \sim \ln^{-1}(a/2Zr_0). \tag{9}$$

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In the real situation, where R-$1 \gtrsim 1$, the accuracy is of order $Z^2\alpha^2$.

The singular matrix element in the operator V is

$$\langle s_{1/2}|V|p_{1/2}\rangle = d(\mathbf{jM})\frac{2}{3}\int\frac{d\mathbf{r}}{4\pi}\left\{\frac{4}{r^3}g_sf_p+\frac{8\pi}{3}\delta(\mathbf{r})(3f_sg_p-g_sf_p)\right\}. \quad (10)$$

Using the identity

$$\frac{d}{dr}(g_sf_p-f_sg_p)=\frac{2}{r^3}g_sf_p, \quad (11)$$

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

$$\langle s_{1/2}|V|p_{1/2}\rangle=-\frac{4\pi}{3}i\,d\mathbf{M}\langle s_{1/2}|\boldsymbol{\gamma}\delta(\mathbf{r})|p_{1/2}\rangle. \quad (12)$$

The identity (12) holds to within a correction term $\sim Z^2\alpha^2/4$. 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[7]). The matrix element $\langle s_{1/2}|\gamma\delta(r)|p_{1/2}\rangle$ contains the above-mentioned relativistic amplification factor R due to the growth of the relativistic wave functions $|s_{1/2}\rangle$ and $|p_{1/2}\rangle$ near the nucleus. A straightforward calculation shows that the matrix element $\langle s_{1/2}|V|p_{3/2}\rangle$ also contains a relativistic amplification factor

$$R_3=\frac{6!\Gamma(\gamma+\gamma_3-2)}{\Gamma(\gamma+\gamma_3+3)\Gamma(\gamma-\gamma_3+3)\Gamma(\gamma_3-\gamma+3)},\qquad \gamma_3=(4-Z^2\alpha^2)^{1/2}. \quad (13)$$

This is closer to unity than is R ($R_3(Xe)=1.29$), since it remains finite as $r_0\to 0$.

The EDM of the xenon atom, subject to the T-odd interaction of the electron with the nucleons,

$$H_T=2i\frac{G}{\sqrt{2}}\Sigma\gamma\delta(\mathbf{r}),\qquad \Sigma=\left\langle C_{Tn}\sum_n\sigma_n+C_{TP}\sum_p\sigma_p\right\rangle \quad (14)$$

was calculated earlier.[2,3] 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 Refs.[2,3] without further calculation. We now need only to take into account the contribution from $p_{3/2}$-electrons, reducing to the substitution $R\to R-R_3\approx R-1$; in the case (14) of pure contact interaction the contribution from the $p_{3/2}$-electrons is absent.

We shall employ this strategy of keeping terms that are singular in r_0, also in calculating the EDM of atoms when we treat simultaneously the hyperfine interaction

$$U=|e|[\mathbf{r}\boldsymbol{\alpha}]\mathbf{M}/r^3 \quad (15)$$

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

$$W=-d\gamma_0\Sigma\mathbf{E}=-\frac{dZ|e|}{r^2}\gamma_0\Sigma\mathbf{n}. \quad (16)$$

Here

$$\boldsymbol{\alpha}=\begin{pmatrix}0&\boldsymbol{\sigma}\\ \boldsymbol{\sigma}&0\end{pmatrix},\qquad \Sigma=\begin{pmatrix}\boldsymbol{\sigma}&0\\0&\boldsymbol{\sigma}\end{pmatrix},\qquad \mathbf{n}=\frac{\mathbf{r}}{r}.$$

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

$$\mathbf{d}_W=\sum_{n,k}\frac{\langle 0|e\mathbf{r}|n\rangle\langle n|U|k\rangle\langle k|W|0\rangle}{(E_0-E_n)(E_0-E_k)}+\ldots, \quad (17)$$

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

$$\mathbf{d}_W'=\sum_n 2\frac{\langle 0|d\gamma_0\Sigma|n\rangle\langle n|U|0\rangle}{E_0-E_n}$$

arising in the second-order approximation has the order of magnitude $d_{W'}\sim Z^{-2}\alpha^2Z^2\alpha^2(m/m_p)d$ 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_0. One may suspect, however, that an r_0-singularity arises in sums of the form

$$\sum_k\frac{\langle n|U|k\rangle\langle k|W|0\rangle}{E_0-E_k} \quad (18)$$

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

We therefore consider the correction

$$|\tilde{0}\rangle=\sum_k\frac{|k\rangle\langle k|W|0\rangle}{E_0-E_k} \quad (19)$$

to the wave function $|0\rangle$ in the region $r\gtrsim r_0$. Applying the operator $H-E_0$ and making use of the completeness condition, we easily arrive at the Dirac radial equations for this correction:

$$f'+\frac{1-\varkappa}{r}f-\frac{Z\alpha}{r}g=\frac{1}{r^2}Z|e|dCZ\alpha r^{\gamma-1},$$
$$g'+\frac{1+\varkappa}{r}g+\frac{Z\alpha}{r}f=\frac{1}{r^2}Z|e|dC(\varkappa-\gamma)r^{\gamma-1}. \quad (20)$$

Here we have omitted the mass and energy of the electron, which are negligible for $r\sim r_0$, and we have also assumed that for small distances we may write the wave function of the ground state in the form.

$$\begin{pmatrix}f_0\\g_0\end{pmatrix}=Cr^{\gamma-1}\begin{pmatrix}\varkappa-\gamma\\Z\alpha\end{pmatrix},\qquad \varkappa=(-1)^{j+1/2-l}. \quad (21)$$

Here j and l refer to the state $|0\rangle$; we note that the orbital moment of the correction $|\tilde{0}\rangle$ is $\tilde{l}=2j-1$. The driven solution of (20) has the form:

$$\begin{pmatrix}f\\g\end{pmatrix}=\frac{Z|e|dC}{2\gamma-1}r^{\gamma-2}\begin{pmatrix}-Z\alpha(2\varkappa-1)\\(\varkappa-\gamma)(2\varkappa+1)\end{pmatrix}. \quad (22)$$

The homogeneous solution $r\gamma^{-1}$ is less singular as $r\to 0$ and at small distances is negligible. A singular homogeneous solution $r^{-\gamma-1}$ 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 $\langle n|U|\tilde{0}\rangle$ is on the order of $Z^2\alpha^2/2$.

It is convenient to introduce the effective operator

$$\tilde{W}=\sum_k\frac{U|k\rangle\langle k|W+W|k\rangle\langle k|U}{-E_k}. \quad (23)$$

By making use of (15), (22), and (21) we see that as $r \to 0$ we have $\tilde{W} \propto U/r \propto 1/r^3$ and the matrix element $\langle s_{1/2}|\tilde{W}|p_{1/2}\rangle$ diverges as $r \to 0$. Using (22) we find, after some simple but rather lengthy transformations,

$$\langle s_{1/2}|\tilde{W}|p_{1/2}\rangle \approx \frac{32\pi}{3}\frac{1}{2\gamma-1} id\mathbf{M}\langle s_{1/2}|\gamma\delta(\mathbf{r})|p_{1/2}\rangle. \quad (24)$$

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

$$\begin{pmatrix} f \\ g \end{pmatrix} = -\frac{4}{3}C|e|\frac{\varkappa \mathbf{M}\mathbf{j}}{2\gamma-1} r^{\gamma-2} \begin{pmatrix} 2(\varkappa+1)(\varkappa-\gamma) \\ Z\alpha(2\varkappa-1) \end{pmatrix}. \quad (25)$$

We note that the terms in (17) containing the matrix elements r between the intermediate states $|n\rangle$ and $|k\rangle$ are negligible since these terms have no singularities with respect to r_0.

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

$$\langle s_{1/2}|V+\tilde{W}|p_{1/2}\rangle \approx \frac{28\pi}{3}\frac{1}{2\gamma-1} id\mathbf{M}\langle s_{1/2}|\gamma\delta(\mathbf{r})|p_{1/2}\rangle. \quad (26)$$

We now note that (17) and (5) 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 $r|0\rangle$. Thus we again find that the contributions of the $p_{1/2}$ and $p_{3/2}$ electrons cancel. We reflect this by substituting $R \to R-1$ in the final solution.

The numerical calculation[3] (cf. also [2]) yields the following expression for the EDM of xenon via the coupling constants (14):

$$d(\mathrm{Xe}) = 0.41 \cdot 10^{-20}|e|\,\text{cm}\,\Sigma. \quad (27)$$

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

$$d(^{129}\mathrm{Xe}) = -1{,}3 \cdot 10^{-3}\frac{R-1}{R}d = -0.8 \cdot 10^{-3} d. \quad (28)$$

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

$$d = (0{,}4 \pm 1{,}4) \cdot 10^{-23}|e| \cdot \text{cm}. \quad (29)$$

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-Fok 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 $^3P_2$ state[8,9]. 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

$$d(^{199}\mathrm{Hg}) = -1.4 \cdot 10^{-2} d. \quad (30)$$

With the aid of the V and $\tilde{W}$ 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[10,11] we find via (26) that

$$d = (0{,}9 \pm 1{,}3) \cdot 10^{-23}|e| \cdot \text{cm}. \quad (31)$$

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 nucleon[1]

$$i\frac{G}{2^{1/2}} k_1 \bar{N} N \bar{e}\gamma_5 e.$$

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

$$H_1 = i\frac{G}{\sqrt{2}} A k_1 \gamma_0\gamma_5\delta(\mathbf{r}),$$
$$k_1 = k_{1p}\frac{Z}{A} + k_{1n}\frac{N}{A}, \qquad N = A - Z, \quad (32)$$

where A 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_1 in a formula of the type of (17). Using (25) for the correction to the wave function due to the HF interaction we find the effective matrix element of the mixture

$$\langle s_{1/2}|\tilde{H}_1|p_{1/2}\rangle = 2i\frac{G}{\sqrt{2}}\Sigma_1\langle s_{1/2}|\gamma\delta(\mathbf{r})|p_{1/2}\rangle,$$
$$\Sigma_1 = \frac{1}{3}\frac{\alpha}{m_p r_0} A k_1 \mu = 4{,}6 \cdot 10^{-4} A^{2/3}\mu k_1. \quad (33)$$

Here μ is the magnetic moment of the nucleus, in nuclear magnetons. We find the finite radius r_0 of the nucleus by using a simple model, assuming that the weak interaction is concentrated entirely in a sphere of radius r_0, and the hyperfine interaction cuts off at a distance much smaller than r_0. This allows us to neglect the homogeneous solution of the inhomogeneous equation for the correction to the wave function arising from the hyperfine interaction. In such a model, as opposed to the model for the EDM of the electron, it is impossible to write an algebraic expression such as $Z^2\alpha^2$ that will characterize the accuracy of the estimate. Nevertheless, this simple model appears to be accurate to within ~50%. Besides, we can if necessary improve the accuracy without too much difficulty, by solving the equation for the hyperfine interaction more accurately. Then, using (1) and (27), we find the bound for the constant k_1

$$k_1 = (0{,}8 \pm 2{,}9) \cdot 10^{-4}. \quad (34)$$

This bound is tighter than the best of the previously existing bounds on the constant $|k_1|$ 5.2 · 10^{-4}, derived from experiments with cesium and xenon in the metastable $^3P_2$ state,[9,13] a very similar bound is derived from an experiment with the TIF molecule:

$$k_1 = (3 \pm 5) \cdot 10^{-4}. \quad (35)$$

To obtain a bound for the constants in a single electron-nucleon T-odd interaction

$$i\frac{G}{\sqrt{2}}k_3\bar{N}\gamma_5 N\bar{e}e$$

we may neglect the HF interaction. In the lowest nonvanishing approximation with respect to m_p^{-1} the corresponding Hamiltonian of the electron-nucleus interaction reduces to the form

$$H_s=-\frac{G}{\sqrt{2}}\frac{1}{2m_p}\left\langle k_{3p}\sum_p \sigma_p+k_{3n}\sum_n \sigma_n\right\rangle \nabla\delta(\mathbf{r})\gamma_0. \quad (36)$$

The matrix element of the mixture is

$$\langle s_{1/2}|H_3|p_{1/2}\rangle\approx 2i\frac{G}{\sqrt{2}}\Sigma_3\langle s_{1/2}|\gamma\delta(\mathbf{r})|p_{1/2}\rangle,$$

$$\Sigma_3=\frac{1}{6}\frac{Z\alpha}{m_p r_0}\left\langle k_{3p}\sum_p \sigma_p+k_{3n}\sum_n \sigma_n\right\rangle. \quad (37)$$

The cesium experiment yields

$$k_{3n}=(-0.3\pm1.1)\cdot10^{-3}, \quad (38)$$

and the TIF experiment yields

$$k_{3p}=(2.5\pm3.8)\cdot10^{-3}. \quad (39)$$

The bounds on the constants k_{3n} and k_{3p} 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

$$\tilde{H}=\frac{G}{\sqrt{2}}\tilde{\varkappa}\delta(r)\frac{\mathbf{I}\alpha}{\mathbf{I}},$$

$$\tilde{\varkappa}=-\frac{1}{3}Q_W\frac{\alpha\mu}{mr_0}=2.5\cdot10^{-4}A^{2/3}\mu. \quad (40)$$

Here I is the spin of the nucleus, $Q_W\approx0.55$, and A is the weak charge of the nucleus. The dimensionless constant $\varkappa$ 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.[14]

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