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НОВОСИБИРСК

NEW LIMITS ON THE ELECTRON DIPOLE MOMENT AND T-NONCONSERVING ELECTRON-NUCLEON INTERACTION

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Abstract

The electric dipole moment (EDM) of an electron together with hyperfine interaction induces EDM in atoms and molecules with closed electron shells. From the experiments with ^{129}Xe and TlF the limits are obtained on the electron EDM ($d/|e|$ = $= (0.4 \pm 1.4)\cdot 10^{-23}$ cm; $(0.9 \pm 1.3)\cdot 10^{-23}$ cm), as well as on the constants of the T-nonconserving scalar electron-nucleon interaction.

In recent experiment [1] very stringent limit on the electric dipole moment (EDM) of ^{129}Xe atom was obtained:

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

From it the limits follow on the constants of T- nonconserving electron-nucleon interaction [2,3] , nucleon-nucleon interaction [3-5] and the proton EDM [3]. In ref. [6] it was noted that due to the hyperfine (HF) interaction the electron EDM can also induce dipole moment in an atom or molecule with closed electron shells, in particular, the xenon atom and TlF molecule. However, no calculation of this effect up to now has been performed.

Such calculation is carried out in the present work. In our opinion, it is interesting by itself from the point of view of atomic theory. The used method of calculation has allowed us also to find the atomic EDM caused by T-odd scalar electron-nucleon interaction. Besides, we have estimated the correction, caused by HF interaction, to T-invariant effects of space parity nonconservation in atoms dependent on nuclear spin.

It is convenient to consider at first the mechanism of atomic EDM that is not connected with HF interaction - the direct interaction of the electron EDM with the nuclear magnetic field. The interaction of the electron EDM d with electromagnetic field $F_{\mu\nu}$ is written in the following relativistically invariant form:

$$H_d = \frac{d}{2}\bar{\psi}\gamma_5\sigma_{\mu\nu}\psi F_{\mu\nu} \qquad (2)$$

Here $\psi = \begin{pmatrix} f\,\Omega_{jl} \\ ig\,\Omega_{j\bar{l}} \end{pmatrix}$, $\bar{\psi} = \psi^+\gamma_0$, f and g are radial wave functions, Ω_{jl} is a spherical spinor, j and l are the total and orbital angular momenta of an electron, $\bar{l} = 2j - l$, $\gamma_5 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$, $\sigma_{\mu\nu} = \frac{1}{2}(\gamma_\mu\gamma_\nu - \gamma_\nu\gamma_\mu)$, γ_μ are Dirac matrices. One can easily obtain from (2) the interaction of an EDM with the magnetic field $\mathcal{H}$ created by nuclear magnetic moment M :

$$V = -i d \vec{\gamma} \vec{\mathcal{H}} \tag{3}$$

$$\vec{\mathcal{H}} = \vec{\nabla} \times [\vec{\nabla} \tfrac{1}{r} \times \vec{M}] = \frac{3(\vec{M}\vec{r})\vec{r} - \vec{M} r^2}{r^5} - \frac{8\pi}{3} \vec{M} \delta(\vec{r}) \tag{4}$$

The expression for the atomic EDM d_V induced by the interaction (3) looks as

$$d_V = \sum_n \frac{\langle 0|V|n\rangle\langle n|e\vec{r}|0\rangle + \langle 0|e\vec{r}|n\rangle\langle n|V|0\rangle}{E_0 - E_n} \tag{5}$$

A naive estimate of expression (5) would give $d_V \sim Z^2\alpha^2 \frac{m}{m_p} d$. The simplest way to see it is to consider the contribution of the last term in (4): $\psi^2(0) \sim Z/a^3$, $\langle\gamma\rangle \sim Z\alpha$, a is the Bohr radius. Take into account, however, that in the non-relativistic limit the operator (3) is proportional to the spin $\vec{\sigma}$:

$$V = -\frac{d}{2m} \vec{\sigma} \left([\vec{p} \times \vec{H}] - [\vec{\mathcal{H}} \times \vec{p}] \right) \tag{6}$$

And since the matrix element of $\vec{r}$ does not act on spin variables, in atoms with closed shells the total spin is equal to zero not only in the ground state $|0\rangle$, but in the intermediate one $|n\rangle$. Therefore, in this limit expression (5) vanishes. More exactly, after the summation over closed shells an additional small factor $\sim Z^2\alpha^2$ should arise in the expression for d_V.

But in fact even at comparatively small $Z^2\alpha^2$ the situation turns out much more favourable. The reason is that under relativistic treatment the matrix element $\langle s_{1/2}|V|p_{1/2}\rangle$ turns to infinity in the limit of a point-like nucleus. When finite nuclear radius r_0 is taken into account, this matrix element contains the relativistic enhancement factor

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

It tends to unity at $Z^2\alpha^2 \to 0$, but even at $Z^2\alpha^2 = 0.16$ (we mean xenon) it is considerably different from unity: $R(Xe) = 2.7$. Enhancement factor in other matrix elements, being non-singular in r_0, are close to unity. Therefore, the compensation of the contributions of closed $p_{1/2}$ and $p_{3/2}$ subshells leads to the factor $R-1$ in the expression for d_V:

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

The factor $R-1$ is not small numerically in xenon although it turns to zero at $Z^2\alpha^2 \to 0$. Below we shall take into account only singular in r_0 terms in the expression for the atomic dipole moment. The expression $R-1$ corresponds to the summation of the leading terms in $\ln(a/2Zr_0)$ in the perturbation theory series in small parameter $Z^2\alpha^2$. Hence, the accuracy of such a calculation at $Z^2\alpha^2 \to 0$ is

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

But in real situation when $R-1 \gtrsim 1$, the accuracy of our calculation is $Z^2\alpha^2$.

The discussed singular matrix element of the operator V equals

$$\langle s_{1/2}|V|p_{1/2}\rangle = d(\vec{J}\vec{M})\frac{2}{3}\int \frac{d\vec{r}}{4\pi}\left\{\frac{4}{r^3} g_s f_p + \frac{8\pi}{3}\delta(\vec{r})(3f_s g_p - g_s f_p)\right\} \tag{10}$$

By means of the identity

$$\frac{d}{dr}(g_s f_p - f_s g_p) = \frac{2}{r^3} g_s f_p \tag{11}$$

that follows from the radial Dirac equation at small distances, the matrix element (10) can be expressed through the matrix element of the operator $\vec{\gamma}\,\delta(\vec{r})$:

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

The identity (12) is valid up to corrections $\sim z^2\alpha^2/4$. Note that with this accuracy the result is independent of the way in which finite nuclear size is taken into account (compare with the calculation of weak interactions in atoms [7]). The matrix element $\langle s_{1/2}\,|\,\vec{\gamma}\,\delta(\vec{r})\,|\,p_{1/2}\rangle$ contains the mentioned above relativistic enhancement factor R due to the increase of relativistic wave functions $|s_{1/2}\rangle$ and $|p_{1/2}\rangle$ near the nucleus. Direct calculation shows that the matrix element $\langle s_{1/2}|V|p_{3/2}\rangle$ also contains a relativistic enhancement factor

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

It is more close to unity than R ($R_3(Xe)=1{,}29$) since it remains finite at $r_0\to 0$.

The EDM of xenon atom caused by T-odd electron-nucleon interaction

$$H_T = 2i\frac{G}{\sqrt{2}}\vec{\Sigma}\vec{\gamma}\,\delta(\vec{r}), \qquad (14)$$

$$\vec{\Sigma} = \langle C_{Tn}\sum_n \vec{\sigma}_n + C_{Tp}\sum_p \vec{\sigma}_p\rangle$$

was calculated previously in refs. [2,3] . It follows from the comparison of formulae (12) and (14) that the xenon EDM can be extracted from the results of refs. [2,3] without further calculations. One should only take into account now the contribution of $p_{3/2}$- electrons, that corresponds to the change

$R\to R-R_3\approx R-1$; in the case of purely contact interaction (14) the contribution of $p_{3/2}$ - electrons is negligible.

The same strategy of looking for the terms singular in r_0 will be followed by us when calculating the atomic EDM arising due to both HF interaction

$$\mathcal{U}=|e|\,\frac{\vec{r}\times\vec{\alpha}}{r^3}\,\vec{M} \qquad (15)$$

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

$$W=-d\gamma_0\vec{\Sigma}\vec{E} = -\frac{dZ|e|}{r^3}\,\gamma_0\vec{\Sigma}\vec{r} \qquad (16)$$

Here

$$\vec{\alpha}=\begin{pmatrix}0&\vec{\sigma}\\ \vec{\sigma}&0\end{pmatrix},\quad \vec{\Sigma}=\begin{pmatrix}\vec{\sigma}&0\\ 0&\vec{\sigma}\end{pmatrix}.$$

The atomic EDM induced by these interactions arises to the third order of perturbation theory

$$d_W=\sum_{n,k}\frac{\langle 0|e\vec{r}|n\rangle\langle n|\mathcal{U}|k\rangle\langle k|W|0\rangle}{(E_0-E_n)(E_0-E_k)} + \text{permutations} \qquad (17)$$

Note immediately that the effect arising to the second order

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

has the order of magnitude $d'_W\sim Z^2\alpha^2\cdot Z\alpha^2\frac{m}{m_p}d$ and is negligibly small in comparison with (8).

The matrix elements of the operators $\mathcal{U}$ and W are by itself non-singular in r_0 . The suspicion however arises that the singularity in r_0 takes place in the sums of the kind

$$\sum_K \frac{\langle n|U|K\rangle\langle K|W|0\rangle}{E_0-E_K} \tag{18}$$

due to the contribution of intermediate states $|K\rangle$ with high energy.

Consider therefore the correction to the wave function

$$|\tilde{0}\rangle = \sum_K \frac{|K\rangle\langle K|W|0\rangle}{E_0-E_K} \tag{19}$$

in the region $r \gtrsim r_0$. Acting on it by the operator $H-E_0$ and using the completeness condition, we get without any difficulty the radial Dirac equations for this correction:

$$\begin{aligned} f' + \frac{1-\varkappa}{r} f - \frac{Z\alpha}{r} g &= \frac{1}{r^2} Z|e|d\, C\, Z\alpha\, r^{\gamma-1} \\ g' + \frac{1+\varkappa}{r} g + \frac{Z\alpha}{r} f &= \frac{1}{r^2} Z|e|d\, C\,(\varkappa-\gamma)\, r^{\gamma-1} \end{aligned} \tag{20}$$

We have neglected here the electron mass and energy, inessential at $r\sim r_0$, and have taken into account also that at small distances the wave function of the state $|0\rangle$ can be written as

$$\begin{pmatrix} f_0 \\ g_0 \end{pmatrix} = C r^{\gamma-1} \begin{pmatrix} \varkappa-\gamma \\ Z\alpha \end{pmatrix} \tag{21}$$

Here $\varkappa = (-1)^{j+\frac{1}{2}-l}$ where j and l refer to the state $|0\rangle$; note that the orbital angular momentum of the correction $|\tilde{0}\rangle$ is $\tilde{l} = 2j-l$. The forced solution of eqs. (20) is

$$\begin{pmatrix} f \\ g \end{pmatrix} = \frac{Z|e|d\,C}{2\gamma-1}\, r^{\gamma-2} \begin{pmatrix} -Z\alpha(2\varkappa-1) \\ (\varkappa-\gamma)(2\varkappa+1) \end{pmatrix} \tag{22}$$

The free solution $r^{\gamma-1}$ is less singular at $r\to 0$ and inessential at small distances. The singular free solution $r^{-\gamma-1}$

arises when boundary conditions at the nucleus are taken into account accurately. But it is essential only in a small vicinity of the nucleus and its relative contribution to the matrix element $\langle n|U|\tilde{0}\rangle$ is of the order of $Z^2\alpha^2/2$.

It is convenient to introduce the effective operator

$$\tilde{W} = \sum_K \frac{U|K\rangle\langle K|W + W|K\rangle\langle K|U}{-E_K} \tag{23}$$

From the comparison of (15), (22) and (21) it can be seen that at $r\to 0$ $\tilde{W} \sim \frac{1}{r} U \sim \frac{1}{r^3}$ and the matrix element $\langle s_{1/2}|\tilde{W}|p_{1/2}\rangle$ diverges at $r_0 \to 0$. By means of (22) we find after simple but rather tedious transformations

$$\langle s_{1/2}|\tilde{W}|p_{1/2}\rangle \approx \frac{32\pi}{3}\frac{1}{2\gamma-1}\, i d\vec{M}\langle s_{1/2}|\vec{\gamma}\,\delta(\vec{r})|p_{1/2}\rangle \tag{24}$$

The same result can be obtained otherwise, by using the equations for the correction to wave function induced by HF interaction. Here the solutions are

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

Note that the terms in expression (17) with matrix elements of $\vec{r}$ between intermediate states $|n\rangle$ and $|K\rangle$ are inessential since these terms have no singularity in r_0. From the comparison of (24) and (12) it follows that the contribution of $\tilde{W}$ dominates numerically. The final value of the matrix element of the mixing equals

$$\langle s_{1/2}|V+\tilde{W}|p_{1/2}\rangle \approx \frac{28\pi}{3}\frac{1}{2\gamma-1}\, i d\vec{M}\langle s_{1/2}|\vec{\gamma}\,\delta(\vec{r})|p_{1/2}\rangle \tag{26}$$

Note now that in non-relativistic limit expression (17), as well as (5), turns to zero for closed electron shells. Indeed, in this limit the sum of the operators W of all the electrons is proportional to their total spin that equals to zero both in the ground state $|0\rangle$ and in the state $\vec{z}\,|0\rangle$. Thus, here again the compensation of the contributions of $p_{1/2}$ and $p_{3/2}$- electrons takes place. We reflect it by the substitution $R \to R-1$ in the final result.

The numerical calculation [3] (see also [2]) have led to the following expression for the xenon EDM through the interaction constants (14):

$$d(Xe) = 0.41 \cdot 10^{-20}\ |e| \cdot cm\ \Sigma \tag{27}$$

From the comparison of the matrix elements (26) and (14), and the result (27) it follows that

$$d\left({}^{129}Xe\right) = -1.3 \cdot 10^{-3}\ \frac{R-1}{R}\ d = -0.8 \cdot 10^{-3} d \tag{28}$$

Using the experimental result (1) we get the limit on the electron EDM:

$$d = (0.4 \pm 1.4) \cdot 10^{-23}\ |e| \cdot cm \tag{29}$$

The theoretical error of this result is caused, first, by the inaccurate account for the terms $\sim Z^2\alpha^2$, and second, by inaccuracy of the Hartree-Fock calculation [3] that have led to formula (27). Therefore, the total error of our calculations does not exceed 30-40%.

The limit (28) is somewhat weaker than the best limits following from the experiments with the atomic cesium and the xenon atom in the metastable state ${}^3P_2$ [8,9]. Note however that the authors of ref. [1] are going to increase the experimental accuracy by four orders of magnitude.

In ref. [1] the possibility is discussed to measure the EDM of mercury where the effects of T-nonconservation are considerably larger. Using the proportionality of the matrix elements (26) and (14) and the calculation with the Hamiltonian (14) for mercury [2], we find

$$d\left({}^{199}Hg\right) = -1.4 \cdot 10^{-2} d \tag{30}$$

By means of the mentioned operators V and $\tilde{W}$ the electron EDM induces as well P- and T- odd dipole moment in a stationary state of polar molecules with paired electrons. Using the limit on the constants in Hamiltonian (14) obtained in the experiments with the molecule TlF [10,11], we find by means of formula (26)

$$d = (0.9 \pm 1.3) \cdot 10^{-23}\ |e| \cdot cm \tag{31}$$

This limit is quite comparable with (29), but the accuracy of the molecular calculations is considerably worse then atomic ones.

Due to HF interaction, the EDM of atoms and molecules with closed electron shells is induced also by the T-odd electron-nucleon interaction $i\frac{G}{\sqrt{2}}k_1\,\bar{N}N\,\bar{e}\gamma_5 e$ [1]. The Hamiltonian of the electron-nucleus interaction in the limit of infinitely heavy nucleon is in this case

$$H_1 = i\frac{G}{\sqrt{2}} A\, k_1\, \gamma_0\gamma_5\, \delta(\vec{z}),$$

$$k_1 = k_{1p}\frac{Z}{A} + k_{1n}\frac{N}{A}, \quad N = A - Z \tag{32}$$

A is an atomic number. The atomic EDM arises here also to the third order of perturbation theory, the only difference being that in the formula of the type (17) H_1 should be substituted for W. Using formula (25) for the correction to wave function caused by HF interaction, we find the effective mixing matrix element

$$\langle s_{1/2} | \tilde{H}_1 | p_{1/2} \rangle = 2i \frac{G}{\sqrt{2}} \Sigma_1 \langle s_{1/2} | \vec{\gamma}\, \delta(\vec{r}) | p_{1/2} \rangle ,$$

$$\Sigma_1 = \frac{1}{3} \frac{\alpha}{m_p r_0} A K_1 \mu = 4.6 \cdot 10^{-4} A^{2/3} \mu K_1 \tag{33}$$

Here μ is the magnetic moment of a nucleus in nuclear magnetons. The finite nuclear radius r_0 is taken into account by means of a simple model: the weak interaction is concentrated on a sphere of the radius r_0 and the HF interaction is cut off near zero at a distance much smaller than r_0. It allows one to neglect the free solutions of inhomogeneous equation for the correction to wave function caused by HF interaction. Unlike the case of the electron EDM, in such a model one cannot write a parameter of the type $Z^2\alpha^2$ that characterizes the accuracy of the calculation. Nevertheless, the accuracy of this simple model is probably about 50%. However, if necessary, it is not so difficult to improve the accuracy of this result by solving more carefully the equation for the HF perturbation.

Now, using (1) and (27), we find the limit on the constant K_1:

$$K_1 = (0.8 \pm 2.9) \cdot 10^{-4} \tag{34}$$

This limit is no worse than the best of previously existing limits on the constant K_1 ($|K_1| < 5.2 \cdot 10^{-4}$) which follows from the experiments with cesium [8,12] and xenon in the metastable $^3P_2$ state [9,13]. A close limit follows from the experiment with the TlF molecule:

$$K_1 = (3 \pm 5) \cdot 10^{-4} \tag{35}$$

To obtain the limits on the constants of another electron-nucleon interaction $i \frac{G}{\sqrt{2}} K_3 \bar{N} \gamma_5 N \bar{e} e$ one should not take into account HF interaction. To the lowest non-vanishing

approximation in m_p^{-1} the corresponding Hamiltonian of the interaction between electron and nucleus is reduced to

$$H_3 = -\frac{G}{\sqrt{2}} \frac{1}{2m_p} \langle K_{3p} \sum_p \vec{\sigma}_p + K_{3n} \sum_n \vec{\sigma}_n \rangle \vec{\nabla} \delta(\vec{r}) \gamma_0 . \tag{36}$$

The mixing matrix element here equals

$$\langle s_{1/2} | H_3 | p_{1/2} \rangle \approx 2i \frac{G}{\sqrt{2}} \vec{\Sigma}_3 \langle s_{1/2} | \vec{\gamma}\, \delta(\vec{r}) | p_{1/2} \rangle ,$$

$$\vec{\Sigma}_3 = \frac{1}{6} \frac{Z\alpha}{m_p r_0} \langle K_{3p} \sum_p \vec{\sigma}_p + K_{3n} \sum_n \vec{\sigma}_n \rangle . \tag{37}$$

From the experiment with xenon it follows

$$K_{3n} = (-0.3 \pm 1.1) \cdot 10^{-3} , \tag{38}$$

from that with TlF

$$K_{3p} = (2.5 \pm 3.8) \cdot 10^{-3} . \tag{39}$$

The limits on the constants K_{3n} and K_{3p} that can be extracted from other experiments are incomparably weaker than (38) and (39).

Note in conclusion that the HF interaction leads also to the dependence on nuclear spin in the matrix element of the T-invariant interaction between electron axial and nucleon vector neutral currents. The corresponding effective operator (compare with (23), (24) and (33)) equals:

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

$$\varkappa = -\frac{1}{3} Q_W \frac{\alpha \mu}{m r_0} = 2.5 \cdot 10^{-4} A^{2/3} \mu \tag{40}$$

Here I is the nuclear spin, $Q_W \approx -0.55A$ is the weak nuclear charge. The dimensionless parameter $\varkappa$ is comparable by magnitude with the corresponding constant that characterizes the interaction of electron vector and nucleon axial neutral currents, but it is by about an order of magnitude smaller than the contribution of the nuclear anapole moment, at least in the case of nonpaired proton [14].

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НОВЫЕ ОГРАНИЧЕНИЯ НА ЭЛЕКТРИЧЕСКИЙ ДИПОЛЬНЫЙ МОМЕНТ ЭЛЕКТРОНА И Т-НЕЧЕТНОЕ ЭЛЕКТРОН-НУКЛОННОЕ ВЗАИМОДЕЙСТВИЕ

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