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abstract

Limit on the proton electric dipole moment (EDM) $|d/e| < 5.5 \cdot 10^{-19}$cm is deduced from the experimental limit on the EDM of atomic cesium in the state with F=4. The analogous measurements for F=3 would allow to improve this result by 1.5 times. From the same experiment the limit on the nucleus magnetic quadrupole moment (it can be induced in particular by the EDM of the valent nucleon) is obtained. Experiments with polar molecules in search for the proton EDM are discussed.

1. Introduction

It is well known[1] that the EDM of elementary particle can exist only if T invariance is not conserved. Up to now T odd interaction was observed evidently only in the decays of K^0 mesons. Hence it is clear that the search for the EDM of elementary particles is of great interest. It is important in particular for the investigation of the structure of T odd interaction.

For the neutron EDM d_n experiment[2] gives the limit $|d_n/e|<10^{-23}$cm. The difficulties with the measurement of the EDM of charged particles - electron and proton - are evident. However, the idea to look for the electron EDM by the neutral atom EDM induced by it appears to be very fruitful. At first sight the situation here seems to be hopeless due to well-known theorem formulated by Schiff[3]. According to this theorem, if the system of non-relativistic particles with EDM is in equilibrium under electrostatic forces, the total EDM of such a system is equal to zero under the condition that the space distributions of charge and dipole moment of every particle coincide. It was shown by Sandars[4] however that the EDM of a heavy atom due to relativistic effects appears to be considerably enhanced in comparison with the electron EDM inducting it. As the computations[4-7] show, this enhancement coefficient constitutes for cesium $K_{Cs}\cong 130$ and for thallium $K_{Tl}\cong 700$. The experiments with atomic cesium[8] and thallium[9] lead to the following limits on the electron EDM: $|d_e/e|<3\cdot 10^{-24}$cm and $|d_e/e|<5\cdot 10^{-24}$cm.

In the present work the limit on the proton EDM is deduced from the experiment with atomic cesium. The limit obtained is perhaps of considerable interest although it is much weaker than the limit that is stated to follow from the experiment with the molecules of TlF[10,11]. The point is that the interpretation[10] does not seem convincing. The limit on the proton EDM from the experiment with TlF can be in fact more weak, say, by an order of magnitude. Moreover, it seems that presently there is no real possibility to extract from this experiment an unambiguous limit on the proton EDM. In detail this question is discussed at the end of the present work.

2. Magnetic quadrupole moment of a nucleus induced by the EDM of the valent nucleon

Begin with the general consideration of the effects due to the EDM of the valent nucleon. The relativistic Hamiltonian of the interaction with an external field $F_{\mu\nu}$ of the dipole moment d belonging to the particle with the spin 1/2 is written as

$$H_d = \frac{d}{2}\gamma_0\gamma_5\sigma_{\mu\nu}F_{\mu\nu}, \qquad \gamma_5 = -i\gamma_0\gamma_1\gamma_2\gamma_3, \qquad \sigma_{\mu\nu} = \frac{1}{2}(\gamma_\mu\gamma_\nu - \gamma_\nu\gamma_\mu) \tag{2.1}$$

The following expressions for the charge and current densities are obtained from (2.1)

$$\rho_d = -d\nabla_n(\Psi^+\gamma_5\gamma_n\Psi) \tag{2.2}$$

$$\underset{\sim}{j}_d = icd\underset{\sim}{\nabla}\times(\Psi^+\underset{\sim}{\gamma}\Psi) \tag{2.3}$$

Pass in them from the Dirac bispinor Ψ to the normalized two-component Schrödinger wave function ϕ restricting to the terms not higher than second order in v/c. Then

$$\rho_d = -d\nabla_n\{\phi^+[\sigma_n - \frac{1}{8m_p^2c^2}(\sigma_n(p'^2+p^2)+2(\underset{\sim}{\sigma}\underset{\sim}{p}')\sigma_n(\underset{\sim}{\sigma}\underset{\sim}{p}))]\phi\} \tag{2.2a}$$

$$\underset{\sim}{j}_d = \frac{d}{2m_p}\underset{\sim}{\nabla}\times[\phi^+\underset{\sim}{\sigma}\times(\underset{\sim}{p}'+\underset{\sim}{p})\phi] \tag{2.3a}$$

Here $\underset{\sim}{p}'$ and $\underset{\sim}{p}$ are momentum operators acting correspondingly on ϕ^+ and ϕ. Begin with the first term in (2.2a) which corresponds to the usual contribution of the valent nucleon to the EDM of the nucleus. Relativistic corrections to the motion of the nucleus as a whole are negligibly small. But then due to the Schiff theorem[3] the nucleus EDM by itself effects the atomic EDM only by means of interaction of the nucleus with the magnetic field created by electrons and by means of the possible effects connected with the finite size of the nucleus. The atom EDM induced by the mentioned magnetic interaction can be shown

to be very small, its order of magnitude is $d\frac{m}{m_p}Z\alpha^2$ (m is electron mass). The consideration of the effects caused by nucleus finite size is postponed to the fourth chapter of the paper.

Relativistic corrections in ρ_d are of two kinds. The first arise because of proton motion in the nucleus and are reduced merely to renormalization of the resulting nucleus EDM. Although they are not so small, but in virtue of the Schiff theorem are of no special interest. The relativistic corrections of the second kind have the structure like $\frac{\hbar^2}{m_p^2c^2}\nabla_k\nabla_m\nabla_n(\phi^+\sigma_k l_m l_n\phi)$ (l is the nucleon orbital momentum) and correspond in particular to the nucleus octupole momentum. The contribution of these corrections to the atomic EDM is also small, it constitutes by an order of magnitude $d(\frac{m}{m_p})^2Z^2\alpha^2$.

Pass now to the consideration of the effects caused by the space current $\underset{\sim}{j}_d$. Simplify the expression (2.3a) using nuclear shell model. For the Cs^{133} nucleus interesting us the errors introduced by this approximation may constitute, if one looks at the Schmidt diagram, about 30-40%. Take at first the expectation value of the operator $\frac{1}{2m_p}(\underset{\sim}{p}'+\underset{\sim}{p})$ in the state of a valent nucleon with a fixed orbital momentum l. We consider in fact the current creating an orbital magnetic momentum. Taking the nucleus as point-like, present corresponding magnetic field as

$$\underset{\sim}{H} = \frac{|e|\hbar}{2m_pc}\underset{\sim}{\nabla}\times[\underset{\sim}{\nabla}\frac{1}{r}\times\underset{\sim}{l}] \tag{2.4}$$

Making use of the Maxwell equation $\underset{\sim}{\nabla}\times\underset{\sim}{H} = \frac{4\pi}{c}\underset{\sim}{j}$ get after simple transformations

$$\overline{\frac{1}{2m_p}(\underset{\sim}{p}'+\underset{\sim}{p})} = \frac{\hbar}{2m_p}\nabla\delta(\underset{\sim}{r})\times\underset{\sim}{l} \tag{2.5}$$

Then

$$\underset{\sim}{j}_d = -d\frac{\hbar}{2m_pc}\underset{\sim}{\nabla}\times[\overline{\underset{\sim}{l}(\sigma\underset{\sim}{\nabla})\delta(\underset{\sim}{r})}] \tag{2.6}$$

Now the bar denotes the expectation value in the state of a nucleus with a fixed total angular momentum i. The tensor $l_m\sigma_n$

can be easily shown to be symmetric and the term with δ_{mn} in it does not contribute evidently to $\underset{\sim}{j}_d$. Accounting for these considerations, obtain

$$j_{d_m} = d\frac{\hbar}{2m_p}\varepsilon_{mrn}\frac{g}{2}[i_r i_s + i_s i_r - \frac{2}{3}\delta_{rs} i(i+1)]\nabla_s\nabla_n\delta(\underset{\sim}{r}) \qquad (2.7)$$

$$g = \frac{1}{4} + \frac{l(l+1)+3/4}{2i(i+1)} - \frac{[l(l+1)-3/4]^2}{i^2(i+1)^2}\cdot\frac{3}{4}$$

For the Cs^{133} nucleus where the state of valent proton is $g_{7/2}$, find $g = -40/189$. Vector-potential, created by the current j_d is equal to

$$A_m = d\frac{\hbar}{2m_p c}\varepsilon_{mrn}\frac{g}{2}[i_r i_s + i_s i_r - \frac{2}{3}\delta_{rs} i(i+1)]\nabla_s\nabla_n\frac{1}{r} \qquad (2.8)$$

Physical interpretation of the effect discussed is evident. As well as orbital motion of a charged particle creates magnetic dipole moment of the system, orbital motion of a particle with EDM creates in the system magnetic quadrupole moment. As an operator of magnetic quadrupole moment in the case considered it is natural to take the tensor

$$M_{mn} = \frac{3}{2}d\frac{\hbar}{m_p c}g[i_m i_n + i_n i_m - \frac{2}{3}\delta_{mn} i(i+1)] \qquad (2.9)$$

Characterize this operator as usually by the quantity

$$M = M_{zz}\Big|_{i_z=i} = d\frac{\hbar}{m_p c}g i(2i-1) \qquad (2.10)$$

For the Cs^{133} nucleus this expression reduces to

$$M_{Cs} = -\frac{80}{9}\frac{d}{|e|}\mu_p \qquad (2.11)$$

where e is electron charge, $\mu_p = \frac{|e|\hbar}{2m_p c}$ is nuclear magneton. Magnetic quadrupole momentum of the nucleus is not evidently equal to zero only if $i \geq 1$.

Note that the formulae (2.5)-(2.10) refer equally to a nucleus with valent neutron possessing EDM, this nucleus also has magnetic quadrupole moment if $i \geq 1$.

3. The atomic EDM induced by magnetic quadrupole moment of nucleus

Relativistic effects in atom are essential, as will be seen below, for the phenomenon discussed. Therefore the Hamiltonian of interaction with the vector-potential $\underset{\sim}{A}$ (see (2.8)) write down directly for relativistic electron:

$$H_1 = d\frac{e\hbar}{2m_p c}\alpha_k\varepsilon_{klm}\nabla_l\nabla_n\frac{1}{r}\cdot\frac{g}{2}[i_m i_n + i_n i_m - \frac{2}{3}\delta_{mn} i(i+1)] \qquad (3.1)$$

where $\underset{\sim}{\alpha} = \gamma_0\underset{\sim}{\gamma}$ is the Dirac matrix for electron.

The ground state of atomic cesium is $6s_{1/2}$. Due to the interaction (3.1) it gets an admixture of the states with the same total atomic momentum F, but with opposite parity. In result atom acquires EDM. Since in cesium the dipole matrix elements 6s-6p are much larger than all others, restrict to the consideration of the admixture of 6p states to the ground state 6s. The electronic part of the interaction (3.1) is evidently an irreducible tensor of the second rank and therefore cannot cause mixture between the states $s_{1/2}$ and $p_{1/2}$ even accounting for relativistic effects. The admixture of the state $6p_{3/2}$ is therefore left.

Relativistic wave functions of electron may be presented as follows

$$\Psi_{s_{1/2}} = \begin{pmatrix} g_{1/2}(r)\Omega_{1/2,0} \\ -if_{1/2}(r)(\frac{\underset{\sim}{\sigma}\underset{\sim}{r}}{r})\Omega_{1/2,0}\end{pmatrix} \qquad \Psi_{p_{3/2}} = \begin{pmatrix} g_{3/2}(r)\Omega_{3/2,1} \\ -if_{3/2}(r)(\frac{\underset{\sim}{\sigma}\underset{\sim}{r}}{r})\Omega_{3/2,1}\end{pmatrix} \qquad (3.2)$$

Here Ω_{jl} is spherical function with spin. Consider radial functions g and f. Due to singular nature of the interaction (3.1) ($\sim r^{-3}$), the main contribution to the matrix element of H_1 is given by the region of small r where the screening of nucleus may be neglected and electronic energy in comparison with potential as well. It can be shown that in this region (see, e.g. [12])

$$rg(r) = -C(\frac{x}{2}\frac{d}{dx} - \varkappa)J_{2\gamma}(x)$$
$$rf(r) = CZ\alpha J_{2\gamma}(x) \qquad (3.3)$$
$$x = (8Zr/a)^{1/2};\quad \varkappa = (-1)^{j+1/2-l}(j+1/2);\quad \gamma = [(j+1/2)^2 - Z^2\alpha^2]^{1/2}$$

$$C = (-1)^{j+1/2-l}(2Ry/e^2\nu^3)^{1/2} \tag{3.4}$$

Here $Ry = \frac{me^4}{2\hbar^2}$ is the Rydberg constant, $a = \frac{\hbar^2}{me^2}$ is the Bohr radius, ν is the effective principal quantum number.

Quite standard, although lengthy, calculation of the matrix element of $s_{1/2}$ and $p_{3/2}$ states mixing in cesium leads to the following result:

$$\langle p_{3/2}|H_1|s_{1/2}\rangle = \frac{d}{ea}\frac{m}{m_p}Z^2\alpha^2 Ry(\nu_p\nu_s)^{-3/2}R\frac{16}{63}\begin{cases}\sqrt{35}\\ -5\sqrt{3}\end{cases} \tag{3.5}$$

Here and below a number in the upper line refers to the total atomic angular momentum F=4 and in the lower one to F=3. Relativistic enhancement factor is equal here to

$$R = \frac{6!\Gamma(\gamma_{1/2}+\gamma_{3/2}-2)}{\Gamma(\gamma_{1/2}+\gamma_{3/2}+3)\Gamma(\gamma_{1/2}-\gamma_{3/2}+3)\Gamma(\gamma_{3/2}-\gamma_{1/2}+3)}=1.3 \tag{3.6}$$

The dipole matrix element of interest is

$$\langle i=7/2,\ j=1/2,\ F;\ F_z=F|ez|i=7/2,\ j=3/2,\ F;\ F_z=F\rangle = ea\rho\begin{cases}\frac{1}{3}\sqrt{7/5}\\ \frac{1}{4}\sqrt{3}\end{cases} \tag{3.7}$$

Making use of (3.5) and (3.7), we get the following expression for the contribution into the EDM of atomic cesium D_1 due to the effect under discussion:

$$D_1 = d\frac{m}{m_p}Z^2\alpha^2\rho\frac{Ry}{E_{6p}-E_{6s}}(\nu_{6s}\nu_{6p})^{-3/2}R\begin{cases}-32/27\\ 40/21\end{cases} \tag{3.8}$$

Being aware of effective quantum numbers $\nu_{6s}=1.87$, $\nu_{6p}=2.35$ and of dimensionless radial matrix element*) $\rho(6s,6p) = -5.8$,

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*) The modulus of ρ is determined from experimental data[13] on oscillator strengths in cesium. The sign of ρ is found from the following considerations. When computing the mixing of s- and p-states, their wave functions were taken positive at $r\to 0$. But then since their radial quantum numbers differ by unity, they have opposite signs at $r\to\infty$. Therefore, the quantity ρ

we come to the following numerical result

$$D_1 = d\cdot 10^{-3}\begin{cases}0.78\\ -1.25\end{cases} \tag{3.9}$$

Comparing (3.9) with the experimental data according to which the EDM of atomic cesium in the state with F=4 $|D_{Cs}/e| < 3.7\cdot 10^{-22}$cm[8], we get the following limit on the proton EDM

$$|d/e| < 4.7\cdot 10^{-19}\text{cm} \tag{3.10}$$

It is almost by four orders of magnitude better than the limit following from the measurement of spin precession of free proton[14]. Note that the limit (3.10) can be improved by 1.5 times if one measures the EDM of atomic cesium in the state with F=3.

And at last, from the experiment with atomic cesium one can extract the limit directly on the magnetic quadrupole moment of the Cs^{133} nucleus. Comparing (2.11) with (3.10) we get

$$|M_{Cs^{133}}| < 6.8\cdot 10^{-6}\mu_p r_{Cs} \tag{3.11}$$

where $r_{Cs}=6.1\cdot 10^{-13}$cm is the radius of the Cs^{133} nucleus. In the report by Sandars[15] the limit by 15 times more weak is mentioned. Since the report[15] does not contain any details, it is impossible to state the cause of such a large disagreement.

4. Atomic EDM caused by the dipole moment of finite-size nucleus

Consider now one more mechanism by means of which the valent nucleon EDM induces the atomic EDM. As it was noted by Schiff[3], even without accounting for relativistic effects the system of particles can possess an EDM if at least for one of them the distributions of charge and EDM do not coincide. The interaction of electron with dipole moment of a finite-size

determined mainly by the behaviour of wave functions at large distances should be negative.

nucleus leading to the atomic EDM may be written as follows

$$H_2 = \int d\underset{\sim}{r}'\,[\rho_d(\underset{\sim}{r}') - \rho_q(\underset{\sim}{r}')]\,\underset{\sim}{d}\cdot\nabla_{\underset{\sim}{r}'}\frac{e}{|\underset{\sim}{r}-\underset{\sim}{r}'|} \qquad (4.1)$$

Here $\underset{\sim}{r}$ is the coordinate of the electron counted off the centre of the nucleus, ρ_d and ρ_q are correspondingly the dipole moment and charge densities of the nucleus each of which is normalized to unity. Restricting to the first non-vanishing term of expansion in r'/r, transform (4.1) to

$$H_2 = \frac{e}{2}\int d\underset{\sim}{r}'\,[\rho_q(\underset{\sim}{r}')-\rho_d(\underset{\sim}{r}')]\,d_l r'_m r'_n \nabla_l\nabla_m\nabla_n\frac{1}{r} \qquad (4.2)$$

The charge density ρ_q is evidently spherically-symmetric up to the corrections of the order Z^{-1}. Even for deformed nuclei where these corrections can be larger by an order of magnitude, they may be nevertheless neglected. As to the quantity ρ_d, it is natural to assume that it coincides with the distribution of valent nucleon. At last, the nucleus dipole moment will be taken as coinciding with this nucleon EDM: $\underset{\sim}{d} = d\underset{\sim}{\sigma}$. Accounting for these remarks, the expression (4.2) may be rewritten as

$$H_2 = \frac{ed}{2}\int d\underset{\sim}{r}'\,r'^2\{\rho_q(r')\tfrac{1}{3}\delta_{mn}\langle\sigma_l\rangle-\rho_d(\underset{\sim}{r}')\langle\sigma_l n_m n_n\rangle\}\nabla_l\nabla_m\nabla_n\frac{1}{r} \qquad (4.3)$$

Here the brackets $\langle\,\rangle$ denote the expectation value in the state with a given nucleus momentum i.

Consider now a cesium atom. Since we are still interested in the mixing of 6s and 6p states, it is sufficient to leave in the "electronic" factor $\nabla_l\nabla_m\nabla_n\frac{1}{r}$ in the interaction its vector part $-\frac{1}{5}(\nabla_l\delta_{mn}+\nabla_m\delta_{ln}+\nabla_n\delta_{lm})4\pi\delta(\underset{\sim}{r})$. Then standard transformations lead in the case of the nucleus Cs^{133} (i=7/2, l=4) to the following expression:

$$H_2 = \frac{1}{189}ed(7r_q^2-3r_d^2)(\underset{\sim}{i}\cdot\underset{\sim}{\nabla})4\pi\delta(\underset{\sim}{r}) \qquad (4.4)$$

What can be said of the mean squares of the radii $r^2_{q,d}= \int d\underset{\sim}{r}'\,r'^2\rho_{q,d}(\underset{\sim}{r}')$? As it is well known, e.g., from electron scattering on nuclei, nuclear charge can be with good accuracy taken as distributed with constant density over the sphere of

of the radius $r_o=1.2\cdot10^{-13}A^{1/3}$cm (A is a mass number of nucleus). Then $r_q^2=0.6r_o^2$. As to the quantity r_d^2 it is natural to assume that it coincides with mean square of magnetic radius of nucleus r_m^2. The last quantity was measured for tritium, He^3, Al^{27}, Sc^{45}, V^{51}, Co^{59}. Since for all these nuclei with the exception of He^3 there is no meaningful difference between r_q^2 and r_m^2 (see the

Table

	$r_q^2\cdot10^{26}cm^2$	$r_m^2\cdot10^{26}cm^2$	$(r_q^2-r_m^2)/r_o^2=\delta r^2/r_o^2$
H_1^3 [16]	2.82±0.34	2.66±0.33	0.03±0.10
He_2^3[16]	3.88±0.40	2.86±0.34	0.16±0.08
Al^{27}_{13}	9.06±0.12[17]	9.18±0.66[18]	-0.01±0.05
Sc^{45}_{21}	12.39±0.63[17]	12.67±1.57[18]	-0.01±0.06
V^{51}_{23}	13.10±0.65[17]	12.89±0.72[18]	0.01±0.05
Co^{59}_{27}	14.21±0.38[17]	13.99±1.05[18]	0.01±0.05

table), take for cesium as well $r_d^2=r_q^2$. Finally we come to the following Hamiltonian of interaction in cesium:

$$H_2 = \frac{4}{315}edr_o^2(\underset{\sim}{i}\cdot\underset{\sim}{\nabla})4\pi\delta(\underset{\sim}{r}) \qquad (4.5)$$

It should be noted that at l≥1 the effect under consideration is caused in fact by orbital quadrupole momentum of nucleus. In distinction from the effect discussed in previous chapters, it depends directly on the radius r_o of nucleus.

The Hamiltonian (4.5) causes the admixture to the ground state $6s_{1/2}$ both $6p_{1/2}$ and $6p_{3/2}$. The admixtures of higher p-states may be neglected again due to the smallness of the corresponding dipole matrix elements. The computation of the same kind as described in the third chapter leads to the following expression for the EDM of atomic cesium induced by the EDM of valent nucleon due to finite size of nucleus:

$$D_2 = d\frac{Z^2 r_0^2}{a^2}\rho\frac{Ry}{E_{6p}-E_{6s}}(\nu_{6s}\nu_{6p})^{-3/2}(R_{1/2}+2R_{3/2})\begin{cases}32/405\\ 8/105\end{cases} \qquad (4.6)$$

Here

$$R_{1/2} = \frac{12\gamma_{1/2}(2r_0Z/a)^{2\gamma_{1/2}-2}}{(2\gamma_{1/2}+1)\Gamma^2(2\gamma_{1/2}+1)} = 2.7 \qquad (4.7)$$

and

$$R_{3/2} = \frac{6[(\gamma_{1/2}+1)(\gamma_{3/2}+2)+Z^2\alpha^2](2r_0Z/a)^{\gamma_{1/2}+\gamma_{3/2}-3}}{\Gamma(2\gamma_{1/2}+1)\Gamma(2\gamma_{1/2}+1)} = 2.2 \qquad (4.8)$$

are the relativistic enhancement factors for the admixture of the states $p_{1/2}$ and $p_{3/2}$ to the ground one. To simplify the formula (4.6) we neglect in it small differences between the energies and dipole matrix elements of the states $6p_{1/2}$ and $6p_{3/2}$.

Comparing the expressions (3.8) and (4.6), we find that the relative magnitude of the EDM of atomic cesium arising due to the finite size of nucleus is sufficiently small:

$$D_2/D_1 = \frac{m_p}{m}(r_0/\alpha a)^2\frac{R_{1/2}+2R_{3/2}}{R}\begin{cases}-1/15\\ 1/25\end{cases} = \begin{cases}-0.17\\ 0.10\end{cases} \qquad (4.9)$$

Therefore, this effect influences weakly the restriction (3.10) obtained in the previous section.

Discuss now the limits on the proton EDM that follow from the experiment with atomic thallium[9]. Both stable isotopes Tl^{203} and Tl^{205} have the angular momentum i=1/2. Hence they cannot possess magnetic quadrupole momentum. According to the shell model valent proton in these nuclei is in the state $s_{1/2}$. Therefore, the interaction (4.3) is reduced for thallium to

$$H_2 = -\frac{1}{3}ed\cdot\delta r^2(\mathbf{i}\cdot\nabla)4\pi\delta(\mathbf{r}), \quad r^2 = r_q^2 - r_d^2 \qquad (4.10)$$

The ground state of atomic thallium is $6s^26p_{1/2}$. Here the dipole matrix elements of the transitions 6p - 7s and 6s - 6p are large. Therefore with sufficient accuracy one may restrict to the consideration of the admixture to the ground state $6s^26p_{1/2}$ of the state $6s^27s$ and the states of the configuration $6s6p^2$. If the total atomic momentum F = 0, the atomic EDM is evidently equal to zero. Consider therefore the states with F = 1.

For the contribution of the $6s^27s$ admixture to the thallium EDM the computation of the kind described above gives

$$D^1 = -\frac{8}{27}d\frac{Z^2\delta r^2}{a^2}\rho(6p,7s)\frac{Ry}{E_{7s}-E_{6p}}(\nu_{7s}\nu_{6p})^{-3/2}R_{1/2} \qquad (4.11)$$

The contribution to the effect of the states of the configuration $6s6p^2$ is conveniently computed by means of the second quantisation technique, its application to a similar problem is described in the work[19]. This contribution is equal to

$$D^2 = -\frac{8}{27}d\frac{Z^2\delta r^2}{a^2}\rho(6s,6p)\frac{Ry}{\bar{E}-E_{6p}}(\nu_{6s}\nu_{6p})^{-3/2}(R_{1/2}+4R_{3/2}) \qquad (4.12)$$

where $\bar{E}$ is the mean energy of the band $6s6p^2$. The relativistic enhancement factors constitute in thallium $R_{1/2} = 7.9$; $R_{3/2} = 4.9$ (see (4.7) and (4.8)). For other parameters the analysis of experimental data on spectra and oscillator strengths in thallium (it is presented in the paper[19]) gives the following values: $\rho(6p_{1/2},7s)=2.2$; $\rho(6s,6p)=-1.7$; $\bar{E}-E_{6p}=71300\,cm^{-1}$; $\nu_{6p}=1.58$; $\nu_{7s}=2.19$; $\nu_{6s}=0.99$.

But in fact, it follows from the comparison of calculated and experimental values of hyperfine structure constants in thallium, as well as from numerical computations of wave functions made by V.V.Flambaum and O.P.Sushkov, that for thallium the normalization coefficient (3.4) and hence the expressions (4.11) and (4.12) are really larger, the last ones approximately two times. Accounting for this circumstance, we find

$$D_{Tl} = 1.8\cdot10^{-3}(\delta r^2/r_0^2)d \qquad (4.13)$$

Any reliable estimate of the quantity δr^2 seems to be very difficult. Calculating the limit on the proton EDM following from the experiment with TlF molecules, Sandars has approximated the potential for valent proton of thallium nucleus with infinite square well of radius r_0 and has obtained in result that $r_q^2-r_d^2=\delta r^2=\frac{4}{15}r_0^2=0.27r_0^2$[10]. The analogous calculation for Sc^{45}, V^{51}, Co^{59} where valent proton is in the state $f_{7/2}$ gives $\delta r^2=0.13r_0^2$ in evident contradiction with experiment (see the table). It is almost evident that these calculations underestimate the value of r_m^2 (or r_d^2) and overestimate correspondingly δr^2. Indeed, the calculations with more realistic Saxon-Wood potential lead, according to communication by V.B.Telitsyn, to $\delta r^2=0.12r_0^2$ for thallium and $\delta r^2=-0.03r_0^2$ for the excited state $f_{7/2}$ in Y^{89}, the last result being at any rate in qualitative agreement with the experimental data presented in the table. However, even this approximation is not sufficiently accurate for our purpose. It is sufficient to make an error about 15-20°/o(and such an error seems to be quite possible in the calculation discussed) and the quantity δr^2 may become smaller again by some times.

It is hardly real presently to determine experimentally r_m^2 for thallium nucleus with its large charge Z=81. Remind that the magnetic moment contribution to electron-nucleus scattering is Z^2 times smaller than charge contribution. It would be very useful in this connection to measure the magnetic radius of F^{19} nucleus, its valent proton being as well as in thallium in the s-state.

Thus, if one takes into account considerably larger accuracy of the experiments with cesium, it can be seen from the formulae (3.9),(4.9) and (4.13) even at the Sandars' value $\delta r^2/r_0^2=0.27$ that atomic thallium is less convenient object for the study of the proton EDM than atomic cesium.

5. Conclusions

Hence, from the experiment with atomic cesium follows, accounting for the correction (4.9), the limit on the proton EDM

$$|d/e| < 5.5\cdot 10^{-19}\text{cm} \qquad (5.1)$$

The largest uncertainty in this result is connected perhaps with using of the shell model when computing magnetic quadrupole moment of nucleus. An error, introduced in this way, may reach 30-40°/o. As to the uncertainty of atomic calculations, if one looks at the analogous computations of hyperfine structure in cesium, it hardly exceeds 15-20°/o.

The limit on the proton EDM following as it is stated from the experiment with TlF molecules[11], is by 35 times more stringent than (5.1). This limit however is grounded essentially on the estimate $\delta r^2/r_0^2=0.27$, this estimate as it was noted in the previous section being perhaps overestimated strongly, and presently no real ways for its improvement are seen. Besides, additional (and evidently ill-controlled) inaccuracy is introduced in computation of molecular wave functions. At any rate, simple estimate of the effective electric field acting on the EDM of valent proton of thallium nucleus in a polarized TlF molecula, leads even at $\delta r^2/r_0^2=0.27$ to value by some times smaller than that given in the works[10,11]. Therefore, the limit on the proton EDM presented in the work[11] seems to be underestimated strongly.

However, the very idea by Sandars on measurement of the proton EDM by means of nuclear magnetic resonance in polar moleculae seems to be very attractive. But more stringent and reliable limits may be perhaps obtained if one uses moleculae with heavy nuclei of moment i> 1/2, e.g., cesium. Such a nucleus may have magnetic quadrupole moment, and therefore the effective electric field acting on the EDM of valent proton will be larger than in the thallium case where it arises only due to the distinction of δr^2 from zero. The advantage is essentially the same that as it was shown above possesses atomic cesium in comparison with atomic thallium.

In conclusion, the following circumstance should be noted. Notwithstanding of the distinction by $2\cdot10^5$ times between the limit (5.1) and the corresponding result for electron ($|d/e| < 3\cdot10^{-24}$ cm[8]), the gap in the physical meaning of these limits may be essentially smaller. The point is that in many models of T-violation (see their review in the work[20]) the EDM of elementary particle is equal to times to its mass (or to the quark mass). But then the proton EDM is by $m_p/m \sim 2\cdot10^3$ times larger than the electron one. Of course, from this point of view the limit on the neutron EDM ($|d/e| < 10^{-23}$ cm[2]) is undoubtedly the leading one. However, the presented considerations should not hypnotize the experimenters since the branch of physics under discussion is only slightly investigated and in it we may come across quite unexpected things.

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