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НОВОСИБИРСК

ON THE POSSIBILITY TO STUDY P- AND T-ODD NUCLEAR FORCES IN ATOMIC AND MOLECULAR EXPERIMENTS

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ABSTRACT

The P- and T-odd nucleon-nucleon potential in the Kobayashi-Maskawa scheme is found. In the shell model analytical expressions for T-odd nuclear multipoles are derived. The electric dipole moments (EDM) of nuclei exceed the neutron EDM by 2-3 orders of magnitude. The EDM of a number of atoms and molecules are calculated. The possible experiments on the search for the T-invariance violation are discussed.

I. Introduction

Although the T-invariance violation [1] was discovered many years ago the decays of neutral K-mesons still remain the only physical phenomena where this effect was observed. This explains a great interest to the search for the electric dipole moments (EDM) of elementary particles, one more possible manifestation of the T-invariance violation [2]. The experiments, being carried out by several groups for a long time (see, e.g., the review [3]), have led to the bounds on the neutron EDM, the most stringent of them being [4]:

$$|d_n/e| < 4\cdot 10^{-25}\,cm \qquad (1)$$

These bounds have reduced drastically the class of possible models of the T-violation.

For the proton EDM the bound considered to be the best one (we shall return to its reliability below) was obtained in the experiments with the TlF molecule [5-7]. If the recent calculations [8] are used, this bound constitutes

$$d_p/e < (2.3 \pm 3.4)\cdot 10^{-21}\,cm \qquad (2)$$

The bound, which follows from the experiment with atomic caesium [9,10] looks as follows [11]:

$$|d_p/e| < 5.5\ 10^{-19}\,cm \qquad (3)$$

The bounds (2) and (3) were derived under the assumption that the EDM of the Tl and Cs nuclei, which have been analysed in the experiments, are due to the EDM of the external proton.

It is difficult however to imagine the situation in which the EDM of the proton and of the neutron, the strongly interacting particles which easily transform into each other virtually (e.g., $n \leftrightarrows p\pi^-$, $p \leftrightarrows n\pi^+$), could differ by several orders of magnitude. For this reason, the impression arises that atomic and molecular experiments on the measurement of the nuclear EDM are of no special interest for elementary-particle physics.

However, from our point of view, it is not true. In the present work we show that the nuclear dipole moment induced by T- and P-odd nucleon-nucleon interaction, can exceed the nucleon EDM by more than two orders of magnitude. An additional enhancement of the nuclear EDM can arise if the nuclear levels of opposite parity are anomalously close. The latter circumstance has been pointed out for the first time in Ref. [12] and discussed in detail quite recently in Refs. [8,13]. However, in our opinion this additional enhancement factor can hardly exceed considerably 10 in stable nuclei. The enhancement of nuclear EDM indicated above drastically diminishes a gap in the sense of available information on the nature of CP-violating interactions between the spectroscopic experiments carried out already and neutron experiments. The possibilities of further advances in atomic and molecular experiments are also discussed in this work.

2. P- and T-odd nucleon-nucleon potential in the Kobayashi--Maskawa model

The progress of the renormalizable theory of electromagnetic and weak interactions provide us with a natural frame to describe CP violation. Two schemes of the kind are discussed most intensively (we do not touch here the models based on grand unification or supersymmetric theories). In one of them CP-violation arises in the Higgs sector of the model [14, 15] and in another in the fermion one [16]. As regards the most popular version of the model of the first kind suggested by Weinberg [15], the neutron EDM following from it [17,18]

$$d_n = -9\cdot 10^{-25}\ e\cdot cm \qquad (4)$$

formally contradicts already the bound (1). There are also indications that this model contradicts also the values of CP violation parameters of $K_L \to 2\pi$ decays [19, 20]. Therefore, we consider P- and T-odd nucleon-nucleon potential in the scheme of CP violation of the second type, the Kobayashi-Maskawa (KM) model [16]. In Refs. [21, 18] it was shown independently that the principal contribution to a neutron EDM is given by the effective operator of the quark-quark interaction

$$H = i\frac{G_1}{\sqrt{2}}\,\bar{s}\,\gamma_\mu(1+\gamma_5)\lambda^a d \sum_{q=u,d}\bar{q}\gamma_\mu\lambda^a q$$

$$G_1 = G\,\sin\delta\; s_1 s_2 s_3 c_2\,\frac{\alpha_s\,\Delta}{12\pi}\,\ln\frac{m_c^2}{m_t^2} \qquad (5)$$

described by the Diagram 1 of the "penguin" type [22] (the dashed line refers to the gluon). Here $G=10^{-5}m_p^{-2}$ is the Fermi weak interaction constant; for the KM matrix and its parameters we follow the convention adopted in Ref. [23], taking $\sin\delta \cdot s_2 s_3 c_2 \sim 10^{-3}$. For the strong interaction constant the value $\alpha_s = 0.2$ is taken. The correction factor Δ which allows for the short-range strong interactions is equal to 1.3 provided the gluons with virtuality from m_t to m_c are taken into account; if we go down to $\mu \sim 0.2$ GeV, Δ amounts to 2.5. This operator is singled out since it contains right-handed currents, their matrix elements being enhanced considerably (see Ref. [22]). Moreover, cancellation of t- and c-quarks contributions in the limit $m_t = m_c$ leads here to the factor $\ln(m_t^2/m_c^2) \sim 6$ instead of the usual one $(m_t^2 - m_c^2)/m_W^2 \sim 0.1$.

The neutron EDM magnitude in the KM model at $\Delta = 1.3$ is equal to [18]

$$d_n = 2\cdot 10^{-32}\ e\cdot cm, \qquad (6a)$$

while at $\Delta = 2.5$

$$d_n = 4\cdot 10^{-32}\ e\cdot cm \qquad (6b)$$

The latter values d_n and Δ are used in the present work. The greater prediction for the neutron EDM $d_n \sim 10^{-30}$ e.cm, obtained in Ref. [21] is perhaps overestimated [24,25].

While constructing the P- and T- odd potential with the help of the operator (5), we retain only pole graphs, avoiding thus at any rate the geometric suppression factors of the type $1/\pi^2$ arising in loops. The simplest diagram of the kind is presented at Fig. 2. The CP-odd vertex denoted with the symbol

$\otimes$ has to be pseudoscalar since just in this case there arises the enhancement of the matrix elements of the operator (5) due to right-handed currents.

Then the CP-even vertex **O** must be scalar, S-wave one.

By means of the standard factorization technique the pseudoscalar part of the matrix element $\langle pK^- | \hat{H} | n \rangle$ can be reduced to the form

$$\frac{G_1}{\sqrt{2}} \frac{4}{9} f_K g_a \frac{m_K^2}{m_s} \frac{2 m_p}{m_u + m_d} \frac{m_\pi^2}{m_\pi^2 - q^2} \bar{P} \gamma_5 n (K^-)^+ \qquad (7)$$

Here f_K = 165 MeV is the constant of $K \to \mu\nu$ decay, g_a = 1.25 is the renormalization constant of axial current, and for the quark current masses we take the values m_s = = 150 MeV, m_d = 7 MeV, m_u = 4 MeV. With the same technique the calculation of the matrix element $\langle \mathcal{N} K^0 | \hat{H} | \mathcal{N} \rangle$, $\mathcal{N} = p, n$, is reduced to the calculation of $\langle \bar{\mathcal{N}} | \bar{d} \gamma_5 d | \mathcal{N} \rangle$. The nucleon matrix element of divergence of the isovector axial current

$$j_{\mu 5}^{(1)} = \frac{1}{2} (\bar{u} \gamma_\mu \gamma_5 u - \bar{d} \gamma_\mu \gamma_5 d)$$

leads to the relation

$$\langle N | m_u \bar{u} \gamma_5 u - m_d \bar{d} \gamma_5 d | N \rangle = g_a m_p \bar{N} \gamma_5 \tau_3 N \frac{m_\pi^2}{m_\pi^2 - q^2} \qquad (8)$$

where $\tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is the isotopic spin operator.

Due to isotopic invariance the matrix element $\langle \mathcal{N} | \bar{u} \gamma_5 u + \bar{d} \gamma_5 d | \mathcal{N} \rangle$ has no π -meson pole and therefore in the chiral limit one obtains

$$\langle \mathcal{N} | m_u (\bar{u} \gamma_5 u + \bar{d} \gamma_5 d) | \mathcal{N} \rangle = 0 \qquad (9)$$

From the formulae (8) and (9) we get

$$\langle \mathcal{N} | \bar{d} \gamma_5 d | \mathcal{N} \rangle = - g_a \frac{m_p}{m_u + m_d} \bar{\mathcal{N}} \gamma_5 \tau_3 \mathcal{N} \frac{m_\pi^2}{m_\pi^2 - q^2} \qquad (10)$$

$$\langle \mathcal{N} K^0 | \hat{H} | \mathcal{N} \rangle = \frac{G_1}{\sqrt{2}} \frac{4}{9} f_K g_a \frac{m_K^2}{m_s} \frac{m_p}{m_u + m_d} \frac{m_\pi^2}{m_\pi^2 - q^2} \bar{\mathcal{N}} \gamma_5 \tau_3 \mathcal{N} \qquad (11)$$

The scalar vertex at Fig. 2 can be expressed through the S-wave amplitudes of non-leptonic hyperon decays. Using the hypothesis of octet dominance we write the S-wave CP-even amplitude of the barion B and pseudoscalar P octets interaction in a form (see, e.g., Ref. [23])

$$A_3 [(PS\bar{B}B) - (SP\bar{B}B)] + A_4 [(PSB\bar{B}) - (SPB\bar{B})] +$$

$$+ A_7 [(S\bar{B})(BP) - (SB)(\bar{B}P)] \qquad (12)$$

Here the spurion $S \sim \lambda_6$ is the sixth component of octet, parentheses mean the trace of a matrix product. The coefficients $A_{3,4,7}$ are expressed through S-wave amplitudes of non-leptonic decays of hyperons in the following way

$$A_3 = -\sqrt{2} A(\Sigma_0^+) = -2.1$$

$$A_7 = A(\Sigma_+^+) = 0.06 \qquad (13)$$

$$A_4 = -\sqrt{\frac{3}{2}} A(\Lambda_-^0) - \frac{1}{\sqrt{2}} A(\Sigma_0^+) = 0.77$$

We use the phase convention of Ref. [22].

Finally, the effective Hamiltonian of the CP-even S-wave interaction of K-mesons and nucleons looks as follows

$$H_w = -iGm_\pi^2\{A_3(\bar P P)(K^0-\bar K^0) +$$

$$+ (A_3 - A_4 + A_7)(\bar n n)(K^0-\bar K^0) +$$

$$+ (A_4 - A_7)[(\bar n P)K^- - (\bar P n)K^+]\} \qquad (14)$$

Note that since the momenta squared of the π -meson in the hyperon decay $(q^2 = m_\pi^2)$ and of the K-meson in the intranuclear exchange are small on the hadronic scale, the coefficients $A_{3,4,7}$ in the expression (14) are close to those of (13) derived from the non-leptonic decays.

Using the formulae (7),(11) and their Hermitean conjugated counterparts as well as (14) we arrive at the following CP-odd Hamiltonian of the nucleon-nucleon interaction

$$\frac{G}{\sqrt{2}}\eta_0\frac{m_\pi^2}{m_\pi^2-q^2}\{i[(\bar P\gamma_5 P)-(\bar n\gamma_5 n)][(\bar P P)+1.34(\bar n n)]-$$

$$-0.34\, i[(\bar P\gamma_5 n)(\bar n P)+(\bar n\gamma_5 P)(\bar P n)]\} \qquad (15)$$

Here η_0 is

$$\eta_0 = G_1 m_\pi^2 \frac{16}{9} g_a \frac{f_K}{m_s}\frac{m_p}{m_u+m_d} A_3 = -0.67\cdot 10^{-8} \qquad (16)$$

The formula (15) was derived under the assumption that the typical momentum transfer in nucleus is much less than m_K, so that K-meson propagator is $(q^2-m_K^2)^{-1}\approx -m_K^{-2}$

The latter term of the formula (15) arising from the charged K-meson exchange reduces after Fierz transformation to the following form in the non-relativistic approximation:

$$-\frac{G}{\sqrt{2}}\frac{\eta_0}{2m}0{,}17[\vec\sigma_p\times\vec\sigma_n](\vec P_{fn}+\vec P_{in}-\vec P_{fp}-\vec P_{ip}) \qquad (17)$$

Here $\vec\sigma_p$ and $\vec\sigma_n$ are the proton and neutron spin operators, $\vec P_i$ and $\vec P_n$ are the initial and final momenta of corresponding particles. In this and following formulae for the sake of simplicity we have omitted a factor $m_\pi^2/(m_\pi^2-q^2)$ leading to non-locality of the interaction in coordinate space. Neither in the usual nucleus where in the shell model the angular momenta of all the nucleons but the outer one are compensated, nor, say, in the deuteron where the total spin is fixed and is not affected by the dipole moment operator, the interaction (17) does not work and, hence below we do not consider it. Curiously enough, in the case of P-odd, but T-even nucleon-nucleon interaction the exchange term with the similar Lorentz structure proves to be essential.

Among other possible mechanisms leading to P- and T-odd nuclear forces in the K M model we have not been able to find any one competing successfully with the K-meson pole exchange. Just this interaction we use below rewriting it in the form

$$\frac{G}{\sqrt{2}}\eta_0 i[(\bar P\gamma_5 P)-(\bar n\gamma_5 n)][(\bar P P)+1.34(\bar n n)] \qquad (18)$$

omitting in the formula (15) the exchange term.

In the heavy nucleus the P- and T-odd interaction of the non-relativistic nucleon with the core is described by the following effective Hamiltonian

$$\hat H = \frac{G}{\sqrt{2}}\frac{\eta}{2m}\vec\sigma\vec\nabla\rho(\vec r) \qquad (19)$$

where σ is the nucleon spin and ρ is the total density of the core protons and neutrons. This phenomenological form of the interaction is not specific to any definite scheme of CP-violation at the level of elementary particles and is thus of a quite general character. In the KM model, of the prime interest to us,

$$\eta_p = -\eta_n = \eta_0 \cdot (1.34 - 0.34\, Z/A) \qquad (20)$$

where Z is the nuclear charge and A is the atomic number. Numerically, at $Z \gtrsim 40$

$$\eta_p = -\eta_n = -0.81 \cdot 10^{-8} \qquad (20a)$$

One should, however, have in mind that the KM model predicts perhaps the smallest values for the constant η and the T-odd multipole moments.

9. The electric dipole and magnetic quadrupole nuclear moments produced by P- and T-odd nucleon-nucleon interaction

The simplest P- and T-odd characteristic of a nucleus is an electric dipole moment (EDM)

$$\vec{d} = e \int \vec{r}\, \delta\rho(\vec{r})\, d^3r = d\, \frac{\vec{I}}{I} \qquad (21)$$

where $\delta\rho$ is a charge density correction induced by the P- and T-odd interaction. However, when the neutral atom or molecule is considered as a system of point-like particles with Coulomb interaction, its total dipole moment vanishes, despite of the presence of a nuclear EDM, by virtue of the well-known Schiff theorem [26] (the detailed consideration of issues related see, e.g., in Ref. [27]). Nevertheless, in the same work [26] it has been noticed that this theorem is violated by taking, in particular, finite size of the nucleus into account. Then it was shown [28], that just this effect mainly causes the violation of the Schiff theorem in heavy atoms and molecu-

les. The Schiff suppression leads to the following form for the P- and T-odd nuclear potential

$$\delta\varphi(\vec{R}) = e \int \frac{\delta\rho(\vec{r})\, d^3r}{|\vec{R} - \vec{r}|} + \frac{1}{Z}(\vec{d}\vec{\nabla}) \int \frac{\rho_0(r)\, d^3r}{|\vec{R} - \vec{r}|} \qquad (22)$$

where $\rho_0(r)$ is a spherical part of the nuclear charge density normalized by the condition $\int d^3r\, \rho_0(r) = Z$. The second term in (22) secures vanishing of a dipole term of potential expansion outside the nucleus in agreement with the Schiff theorem. The total atomic or molecular EDM in this case is merely that of electron shells, induced by the potential (22). When calculating the nuclear EDM or the potential (22), in addition to the motion of the external nucleon one has to take into account the nuclear core motion. It is well-known that even in a heavy nucleus its large mass is compensated by the large charge. Let $\delta\rho_v$ be the T- and P-odd correction to probability density connected with an external nucleon. Then the whole correction to the charge density $\delta\rho$ of formulae (21) and (22) is written as

$$\delta\rho(\vec{r}) = q\, \delta\rho_v + \frac{1}{A} \nabla\rho_0(r) \langle \vec{r} \rangle \qquad (23)$$

where $q = 0,1$ for a neutron and proton respectively, $\langle \vec{r} \rangle$ is the contribution to the dipole moment of a nucleus owing to an unpaired nucleon

$$\langle \vec{r} \rangle = \int \delta\rho_v(\vec{r})\, \vec{r}\, d^3r \qquad (24)$$

The second term in (23) takes it into account that when the external nucleon moves, the core is shifted also relatively to the centre of mass ($\vec{r}_c \approx -\vec{r}/A$) which leads to the change of the charge density

$$\rho_0(\vec{r} - \vec{r}_c) - \rho_0(\vec{r}) \approx \frac{1}{A}\, \vec{r}\, \vec{\nabla}\rho_0(r)$$

With the recoil effect (23) taken into account, the nuclear EDM takes, as it should be expected, the form

$$\vec{d} = e\left(q - \frac{Z}{A}\right)\langle \vec{r} \rangle \qquad (25)$$

With the aid of the formula (23) one easily checks the mutual cancellation of recoil effects in the expression (22) for $\delta\varphi$:

$$\delta\varphi(\vec{R}) = eq\left\{\int \frac{\delta\rho_v(\vec{r})}{|\vec{R}-\vec{r}|} d^3r + \frac{1}{Z}\langle \vec{r} \rangle \frac{\partial}{\partial \vec{R}} \int \frac{\rho_0(r)}{|\vec{R}-\vec{r}|} d^3r\right\} \qquad (26)$$

Thus $\delta\varphi$ has a simple form as if the recoil effect were absent. The potential (26) can be expanded in powers of $1/R$

$$\delta\varphi(\vec{R}) = eq\left\{-\frac{1}{6}\int \delta\rho_v(\vec{r})\, r_n r_m r_e d^3r + \right. \qquad (27)$$

$$\left. + \frac{1}{2}\langle r_m \rangle \int \frac{\rho_0}{Z} r_n r_e d^3r \right\} \partial_m \partial_n \partial_e \frac{1}{R} + \ldots$$

Take into account the relation

$$\partial_m \partial_n \partial_e \frac{1}{R} = \left[\partial_m \partial_n \partial_e - \frac{1}{5}(\delta_{mn}\partial_e + \delta_{me}\partial_n + \delta_{ne}\partial_m)\partial^2\right]\frac{1}{R} + \qquad (28)$$

$$+ \frac{1}{5}(\delta_{mn}\partial_e + \delta_{me}\partial_n + \delta_{ne}\partial_m)\partial^2 \frac{1}{R}$$

The term in the square brackets is an irreducible tensor of the third rank (octupole). We do not consider it since the corresponding interaction brings about the mixing of atomic states only with high angular momenta so that its contribution to an atomic or molecular EDM is suppressed considerably. The

dipole remainder in $\delta\varphi$ looks as follows

$$\delta\varphi = -Q_m \partial_m \Delta \frac{1}{R} = 4\pi Q_m \partial_m \delta(\vec{R})$$

$$H_{TP} = -e\delta\varphi = -4\pi e Q_m \partial_m \delta(\vec{R}) \qquad (29)$$

$$Q_m = \frac{eq}{10}\left[\int \delta\rho_v r^2 r_m d^3r - \frac{5}{3}\langle r_m \rangle r_q^2\right] = Q\frac{I_m}{I}$$

Here H_{TP} is the Hamiltonian of the T- and P-odd interaction between a nucleus and electron and $r_q^2 = \frac{1}{Z}\int \rho_0 r^2 d^3r$ is the mean square of the nuclear charge radius. Below we shall call the quantity Q nuclear Schiff moment.

The T- and P-violating interaction between an electron and nucleus arises also due to a nuclear magnetic quadrupole moment (MQM) [11]. In the gauge $div\vec{A} = 0$, the expansion in powers of $1/R$ of the vector-potential, produced by stationary current density, has the form

$$A_i(\vec{R}) = \int \frac{j_i(\vec{r})d^3r}{|\vec{R}-\vec{r}|} = -\int j_i r_m d^3r\, \partial_m \frac{1}{R} + \frac{1}{2}\int j_i r_m r_n\, d^3r \partial_m \partial_n \frac{1}{R} + \ldots \qquad (30)$$

The first term of the expansion corresponds to a magnetic dipole and we have no interest in it. Let us transform the second term taking into account the equation derived from the current conservation $(\partial_n j_n = 0)$:

$$0 = \int \partial_p (j_p r_m r_n r_k) d^3r = \int [j_m r_n r_k + j_n r_m r_k + j_k r_m r_n] d^3r \qquad (31)$$

Since $\langle j_i r_m r_n \rangle$ is multiplied by the tensor symmetrical in indices n, m, we replace

$$\frac{1}{2}\langle j_i r_m r_n\rangle \to \frac{1}{3}\langle (j_i r_m - j_m r_i) r_n\rangle \qquad (32)$$

The expansion of the right hand side in a sum of irreducible tensor is

$$\frac{1}{3}\langle (j_i r_m - j_m r_i) r_n\rangle = \varepsilon_{imk}\left(\frac{1}{4\pi}\varepsilon_{kne} a_e - \frac{1}{6} M_{kn}\right) \qquad (33)$$

where a_e is a vector and M_{kn} is a symmetrical tensor.

It is not difficult to find an explicit form for a_e and M_{kn} from equation (33)

$$a_e = -\pi \int j_i r^2 d^3 r \qquad (34)$$

$$M_{kn} = -\int (r_k \varepsilon_{npq} + r_n \varepsilon_{kpq}) j_p r_q d^3 r$$

The vector potential A is expressed through a and M in the following way

$$A_i = \left[\frac{1}{4\pi}(\delta_{ik} a_e - \delta_{ek} a_i) - \frac{1}{6}\varepsilon_{ien} M_{nk}\right]\partial_e \partial_k \frac{1}{R} \qquad (35)$$

The quantity a is an anapole moment of the system and M is a magnetic quadrupole moment. For the quantum system in a state with a definite angular momentum $\vec{I}$

$$\vec{a} = a\frac{\vec{I}}{I}$$

$$M_{mk} = \frac{3}{2}\frac{M}{I(2I-1)}\left[I_m I_k + I_k I_m - \frac{2}{3} I(I+1)\delta_{mk}\right] \qquad (36)$$

Comparing (34) and (36), we see that an anapole moment arises due to spatial parity violation while the time parity is conserved, and the MQM arises from both the P- and T-violation. An anapole moment of nuclei was considered earlier in the paper [29]. In this paper we deal only with the P- and T-odd effects.

The electromagnetic current of a nucleon in the non-relativistic limit has the form

$$\vec{j} = \frac{ie}{2m} q(\psi\vec{\nabla}\psi^* - \psi^*\nabla\psi) + \frac{e\mu}{2m}\vec{\nabla}\times\psi^*\vec{\sigma}\psi \qquad (37)$$

where m, μ is the mass and the magnetic moment of a nucleon in nuclear magnetons. In (37) we have neglected weak dependence of nuclear forces on velocity.

Substituting (37) into (34) we find

$$M_{kn} = \frac{e}{2m}\langle 3\mu(r_k\sigma_n + r_n\sigma_k - \frac{2}{3}\delta_{kn}\vec{\sigma}\vec{r}) +$$

$$+ 2q(r_k l_n + r_n l_k)\rangle \qquad (38)$$

a) The spherical nuclei

Consider spherical nuclei with a single unpaired nucleon. Taking into account the T- and P-odd interaction, the wave-function of an outer nucleon has the form

$$\tilde{\Psi}_{Im} = R_0(r)\Omega_{Ilm} + \beta R_1(r)\tilde{\Omega}_{Ilm}, \qquad (39)$$

Ω is a spherical spinor [30], $\tilde{\Omega} = -\vec{\sigma}\frac{\vec{r}}{r}\Omega$, β is a real mixing coefficient. With the aid of formulae (25), (29), (38) and (39) we find

$$d = -\frac{1}{2(I+1)} e\left(q - \frac{Z}{A}\right)\langle r\rangle$$

$$Q = -\frac{eq}{20(I+1)}\left(\langle r^3\rangle - \frac{5}{3} r_q^2 \langle r\rangle\right) \qquad (40)$$

$$M = \frac{2I-1}{I+1}\frac{e}{2m}(\mu - q)\langle r\rangle$$

Here

$$\langle r^n\rangle \equiv 2\beta \int R_0 R_1 r^{n+2} dr$$

Note that according to (40) the MQM arises only due to the existence of a nucleon anomalous magnetic moment. Quite easily one can check it using the Dirac equation in the spherical potential. In the case of a non-spherical nucleus, the normal magnetic moment contribute to the MQM as well. It is curious

that by the same reason the atomic MQM induced by an electron EDM in the central field approximation will contain an additional small parameter - the electron anomalous magnetic moment $\alpha/2\pi$. At the same the molecular MQM induced by an electron EDM has no such suppression.

Using the Hamiltonian (19) one can calculate the mixing coefficient β and quantities $\langle r^3\rangle$, $\langle r\rangle$, for example, with Saxon-Woods potential. To start with, we perform the calculations in a simple model allowing an analytical solution, such a calculation being in fact no less accurate than the numerical one. Consider the motion of an unpaired nucleon in the nuclear potential U neglecting the spin-orbit interaction. The shape of the nuclear density ρ and potential U is known to be rather similar. Suppose that they coincide exactly: $\rho_0(r) = U(r)\rho_0(0)/U(0)$. Then one can rewrite (19) in a form

$$H_{TP} = \xi \vec{\sigma}\vec{\nabla}U, \quad \xi = \eta\frac{G}{2\sqrt{2}m}\frac{\rho_0(0)}{U(0)} = -2\cdot 10^{-21}\eta\ cm \qquad (42)$$

Correspondingly, the whole potential affecting the nucleon motion is equal to

$$\tilde{U} = U + H_{TP} = U + \xi\vec{\sigma}\vec{\nabla}U \approx U(\vec{r} + \xi\vec{\sigma}) \qquad (43)$$

Hence it is obvious that the wave-function with H_{TP} taken into account has the form

$$\tilde{\Psi} = \Psi(\vec{r} + \xi\vec{\sigma}) = (1 + \xi\vec{\sigma}\vec{\nabla})\Psi(\vec{r}) \qquad (44)$$

where $\Psi(\vec{r})$ is a non-perturbed wave-function. With the aid of (44), as well as (25),(29) and (38), we find

$$d = -e\left(q - \frac{Z}{A}\right)\xi t_I \qquad (45)$$

$$Q = -\frac{eq}{10}\xi\left[\left(t_I + \frac{1}{I+1}\right)\overline{r^2} - \frac{5}{3}t_I r_q^2\right] \qquad (46)$$

$$M = \frac{e}{m}(\mu - q)(2I-1)t_I \xi \qquad (47)$$

where $\overline{r^2} = \int |\psi|^2 r^2 d^3r$ is a mean square radius of an unpaired nucleon

$$t_I = \begin{cases} 1 & I = l + \frac{1}{2} \\ -\frac{I}{I+1} & I = l - \frac{1}{2} \end{cases} \qquad (48)$$

and l is the orbital angular momentum of a nucleon.

The numerical calculation with Saxon-Wood potential and the experimental data on electric and magnetic radii of nuclei show that the values $\overline{r^2}$ and r_q^2 are close to each other and one can take $\overline{r^2} = r_q^2 = \frac{3}{5}R^2$, $R = r_0 A^{1/3}$ being the nuclear radius ($r_0 = 1.1$ f m) . Then

$$Q \approx -eq\left[t_I - \frac{3}{2(I+1)}\right] A^{2/3} \cdot 10^{-9} \eta \cdot (fm)^3 \qquad (49)$$

Note that the d and M do not depend on A while Q increases as $A^{2/3}$.

It is interesting to compare parametrically the values of the nuclear EDM d and that of a neutron d_n . In general it is possible only for a definite scheme of CP violation. However, there exist a rather regular factor enhancing d compared with d_n.

$$\frac{d}{d_n} \sim (m_\pi^2 U r_0^3)^{-1} 3\pi \approx 60 \qquad (50)$$

Here the factor $(m_\pi^2 U r_0^3)^{-1}$ is of quite an obvious nuclear origin. The factor 3π , being of geometric origin, arises when d appears in a tree approximation while

d_n only in a single-loop one. An enhancement factor additional to (50) in the KM model is of quite accidental numerical character. In the scheme where CP-violation is caused by θ-term (corresponding contribution to the P- and T-odd nuclear multipoles has been considered in the work [13]) additional numerical factors result not in increase, but in noticeable decrease of the (50).

As one can see, for the $S_{1/2}$-nucleon ($l=0$, $I=1/2$) the formula (49) yields Q = 0. The matter is that we have taken $\overline{r^2} = r_q^2$ while according to (46) in this case

$$Q = -\frac{eq}{6}\xi(\overline{r^2} - r_q^2) \qquad (51)$$

i.e. there takes place strong cancellation of two terms. Note that this is the same situation as for the contribution induced by the proton intrinsic dipole moment [28]. It is clear that here at the strong compensation the above model, allowing analytical solution, provides us only with an-order-of-magnitude estimate for Q. Of practical importance are ^{203}Tl and ^{205}Tl, where experimental data are available (see below). The numerical calculation with the Saxon-Woods potential using the formulae (39),(40) yields

$$Q_{Tl} \approx -2 \cdot 10^{-8} \eta e (fm)^3 \qquad (52)$$

The similar calculation by formula (51) gives $-1.3 \cdot 10^{-8}$. The result (52) is also of no high accuracy, since, according to V.B.Telitsin calculations [31], the difference $\overline{r^2} - r_q^2$ is very sensitive to polarization effects and even can change its sign if they are taken into account accurately (with the Saxon-Woods potential, $(\overline{r^2} - r_q^2)/r_q^2 = -0.13$ while Ref. [13] gives 0.07 ± 0.13).

As regards the other nuclei, numerical calculations with Saxon-Woods potential show that the accuracy of formulae (45), (46),(47) and (49) is ~ 50 per cent. Since this accuracy is comparable to that of a shell model, the further refinement of

the formulae (45)-(49) is reasonable only together with taking into account the many-body effects in a nucleus. As the numerical calculations show, the corrections $\sim$ 50 per cent can arise from non-locality of the nucleon-nucleon T- and P-odd interaction ($\Delta r \sim 1/m_\pi$) .

According to the formulae (46) and (49), in the shell model for nuclei with an external neutron ($q=0$) the Schiff moment Q is equal to zero. Due to the core polarization, for a neutron $q \sim 0.1$, so that Q does not vanish in this case too.

The numerical values of d , Q , M for some nuclei are presented in Table 1.

b) <u>Non-spherical nuclei</u>.

The non-spherical nuclei are known to have opposite parity levels close to each other. This fact results in enhancement of effects connected with the usual weak interaction. The possibility of enhancement of the EDM of non-spherical nuclei due to the ground state being accompanied by a close level of opposite parity with the same angular momentum has been pointed out for the first time in Ref. [12] and discussed quite recently in Refs. [8,13]. Unfortunately, among the heavy stable nuclei the choice is scarce. Actually, there is ^{161}Dy with a level $|5/2^-\rangle$ being 25.7 KeV above the ground state $|5/2^+\rangle$, and also ^{237}Np (the ground state $|5/2^+\rangle$, the excited one $|5/2^-\rangle$, ΔE = 59.5 KeV). There are some more nuclei with $\Delta E \sim$ 100 KeV (^{153}Eu, ^{155}Gd, ^{163}Dy, ^{233}U). At first sight, one can expect a significant enhancement of the effects, as compared with spherical nuclei where $\Delta E \sim$ 8 MeV. However, the enhancement factor for the nuclei listed can hardly exceed considerably 10.

For deformed nuclei the calculation is carried out in a "frozen" frame (rotating together with a nucleus). The transition into laboratory frame is performed by the formulae

$$d_{lab} = \frac{J}{J+1} d_z \ , \quad Q_{lab} = \frac{J}{J+1} Q_z \ ,$$

$$M_{lab} = \frac{J}{J+1} \frac{2J-1}{2J+3} M_{zz} \qquad (53)$$

We take into account that in the ground state of a rotational band $J=\Omega$, Ω is an angular momentum projection on a nuclear axis. The quantities d_z , Q_z , M_{zz} are the components of respective tensors in a frozen frame, the axis z is directed along the nuclear axis. The contribution corresponding to a nearby level is equal to

$$T = 2 \frac{\langle \Omega | H_{TP} | \bar{\Omega} \rangle \langle \bar{\Omega} | \hat{T} | \Omega \rangle}{E_\Omega - E_{\bar{\Omega}}} \qquad (54)$$

where $T = d_z$, Q_z , M_{zz} is an operator under consideration, $|\Omega\rangle$ is the ground state and $|\bar{\Omega}\rangle$ is the state of opposite parity. The calculation of matrix elements in the formula (54) has been carried out with the Nilsson one-particle oscillator model. Unfortunately, matrix elements between nearest levels are small and calculations are quite unreliable. For example, the calculated matrix element $\langle 5/2^+ | \hat{d}_z | 5/2^- \rangle$ is five times less than the experimental one derived from the lifetime of a $|5/2^-\rangle$ level of ^{161}Dy. The matrix element $\langle \Omega | H_{TP} | \bar{\Omega} \rangle$ turns out to be also strongly dependent on the choice of parameters of density distribution ρ in Hamiltonian (19). Only the matrix element $\langle \bar{\Omega} | \hat{M}_{zz} | \Omega \rangle$, being not small, can be calculated reliably. There are regular reasons of suppression of matrix elements of d_z , Q_z , H_{TP} . First, the angular momenta I , I' of components dominating in the Nilsson functions of anomalously close states differ from each other by two units and therefore these components are not mixed by the operators listed above. Second, for the operator H_{TP} there is a specific reason for the suppression connected with its spatial structure. The similarity of a shape of density and that of potential occurs in non-spherical nuclei as well. Therefore, when spin-orbit interaction is neglected, the approximate formula (42) is true:

$H_{TP} \approx \xi \vec{\sigma} \vec{\nabla} U = i \xi [\vec{\sigma} \vec{p}, H_0]$, where

$H_0 = p^2/2m + U$ is the one-particle Hamiltonian.
Therefore one obtains

$$\langle \Omega | H_{TP} | \bar{\Omega} \rangle = i\xi \langle \Omega | [\vec{\sigma}\vec{P}, H_0] | \bar{\Omega} \rangle \sim$$

$$\sim E_{\bar{\Omega}} - E_{\Omega} \qquad (55)$$

In a similar fashion the reason for anomalous suppression of $\langle \Omega | \hat{d}_z | \bar{\Omega} \rangle$ calculated by the Nilsson oscillator model can be understood. Really, if $U = \frac{m\omega_1^2(x^2+y^2)}{2} + \frac{m\omega_z^2 z^2}{2}$ then

$$d_z = e r_z = \frac{e}{m\omega_z^2} \frac{\partial U}{\partial z} = \frac{ie}{m\omega_z^2} [P_z, H_0] \qquad (56)$$

Consequently, $\langle \Omega | \hat{d}_z | \bar{\Omega} \rangle$ is proportional to the small difference of energies $E_{\bar{\Omega}} - E_{\Omega}$ as well.

Thus, applying the formulae (55),(56) literally one obtains, according to (54), that the contribution of the anomalously close state to M_{zz} and Q_z has no enhancement, and for d_z it is even suppressed. In fact, it is not true, since the spin-orbit interaction cannot be disregarded and there is no complete similarity between potential and density shapes. The numerical calculations in the Nilsson model lead to the following conclusions. The enhancement of d and Q as compared with spherical nuclei is absent when calculated values $\langle \Omega | d_z | \bar{\Omega} \rangle$ are used. However, with experimental values in use the EDM in ^{161}Dy turns out to be 5÷10 times enhanced (in ^{237}Np the experimental value is two times smaller than the calculated one). The magnetic quadrupole in ^{161}Dy and ^{237}Np turns out to be enhanced by about an order of magnitude. The calculation results are given in Table 1. We stress once more that

for the deformed nuclei our calculations are only an-order-of-magnitude estimates of d, Q and M values. They probably can be improved using deformed Saxon-Woods potential.

c) Light nuclei: ^{2}H, ^{3}He

The binding energy of deuteron is relatively small, $E \approx -2$ MeV. Therefore, the wavefunction size is much greater than the radii of both strong and weak (T- and P-odd) interactions. A non-perturbed wave-function outside the range of nuclear forces is

$$\Psi = \chi_s \sqrt{\frac{\varkappa}{4\pi}} \frac{e^{-\varkappa r}}{r} \qquad (57)$$

where $\varkappa = \sqrt{2m|E|}$ and χ_s is the spin wavefunction ($S = 1$). With T- and P-odd interaction (18)-(20) taken into account the wavefunction in the outer region is

$$\tilde{\Psi} = \left[1 - \gamma \frac{G}{16\sqrt{2}a} (\eta_1 \vec{\sigma}_p - \eta_2 \vec{\sigma}_n) \vec{\nabla}\right] \Psi \qquad (58)$$

where a is the nuclear forces range, $\vec{\sigma}_p$, $\vec{\sigma}_n$ are Pauli matrices for a proton and neutron and γ is a dimensionless numerical factor. In the K M model, $\eta_1 = 1.34\,\eta_0$, $\eta_2 = -\eta_0$. The formula (58) can be derived under various model assumptions, for example, for square-well potential. The γ parameter depends on the model, however, in all the cases considered $\gamma \sim 1$. Note that no suppression of a wavefunction correction arises from the small binding energy of the deuteron. With the help of (58) we find

$$d = \frac{\gamma e G}{32\sqrt{2}a} (\eta_1 - \eta_2)$$
$$Q = 0 \qquad (59)$$
$$M = -\frac{\gamma G}{16\sqrt{2}a} (\mu_p \eta_1 + \mu_n \eta_2) \frac{e}{m_p}$$

where μ_p, μ_n are magnetic moments of proton and neutron in the nuclear magnetons. The numerical values of d, Q and M at $a = 1\,fm$ are given in Table 1. The values of d and M are seen to be practically the same as in heavy spherical nuclei. In the same Table 1 estimates for ^{3}He are given which are obtained by means of formulae (46),(47).

4. Electric dipole moments of atoms and molecules

a) One-particle matrix elements between electron-states.

The Hamiltonian of interaction of an electron with a magnetic quadrupole field (36) has a form

$$H_M = -\frac{Me}{4I(2I-1)}\, t_{mk}\, A_{mk}$$
$$t_{mk} = I_m I_k + I_k I_m - \frac{2}{3}\delta_{km} I(I+1) \qquad (60)$$
$$A_{mk} = \varepsilon_{nim}\, \alpha_n\, \partial_i \partial_k \frac{1}{r}$$

Here I is the nuclear angular momentum, α_n is the Dirac matrix for an electron. The matrix element of H_M between one-electron states is equal to

$$\langle \Psi_2 | H_M | \Psi_1 \rangle = -\frac{3}{8}\frac{eMS}{I(2I-1)}\cdot$$
$$t_{mk} \langle \Omega_2 | \partial_m n_k + \partial_k n_m - 2(\vec{\partial}\vec{n}) n_k n_m | \Omega_1 \rangle \qquad (61)$$

where Ω is a spherical spinor corresponding to a total electron angular momentum j, $\vec{n} = \vec{r}/r$. The radial integral can be calculated with the help of quasiclassical wavefunctions given, for example, in [27]

$$S = \int \frac{1}{r^2}(f_2 g_1 + f_1 g_2)\, dr \approx X \frac{Z_i^2 Z^2 \alpha}{a_B^3 \sqrt{\nu_1^3 \nu_2^3}} R_M \qquad (62)$$

$$X = \frac{\varkappa_1 \varkappa_2}{|\varkappa_1 \varkappa_2|} \frac{96(\varkappa_1+\varkappa_2-2)(j_1+j_2-2)!}{(j_2-j_1+2)!\,(j_1+j_2+3)!\,(j_1-j_2+2)!} \qquad (63)$$

$$R_M = \frac{(j_2-j_1+2)!\,(j_1+j_2+3)!\,(j_1-j_2+2)!\,\Gamma(\gamma_1+\gamma_2-2)}{(j_1+j_2-2)!\,\Gamma(\gamma_2-\gamma_1+3)\Gamma(\gamma_1+\gamma_2+3)\Gamma(\gamma_1-\gamma_2+3)} \qquad (64)$$

where $\varkappa = (j+1/2)\cdot(-1)^{j+\frac{1}{2}-\ell}$, $\gamma = \sqrt{(j+\frac{1}{2})^2 - (Z\alpha)^2}$; a_B is the Bohr radius; f, g are upper and lower radial components of the electron bispinor, Z_i is the atomic core charge and ν is the effective principal quantum number for an external electron ($E = -Z_i^2 Ry/\nu^2$, $Ry = e^2/2a_B$). The relativistic factor R_M is defined so that $R_M \to 1$ at $Z\alpha \to 0$. In the most important case of the $S - P_{3/2}$ matrix element, the numerical factor $X = -2/3$, $R_M(Z=55) = 1.3$, $R_M(Z=80) = 1.8$. In a similar way the calculations are done for the matrix element of interaction of an electron with the scalar T- and P-odd potential of a nucleus (22),(29). Here one has to take into account the mixing of the S- and P- waves only since for higher angular momenta of an electron there arises the suppression $\sim RZ/a_B$, R is a nuclear radius. Using formula (22) we find

$$\langle S | H_{TP} | P \rangle = \frac{4 Z_i^2 Z^2 e R_Q}{a_B^4 \sqrt{\nu_S^3 \nu_P^3}} \vec{Q} \langle \Omega_S | \vec{n} | \Omega_P \rangle \qquad (65)$$

The relativistic factor R_Q is different for the $P_{1/2}$- and $P_{3/2}$ -electrons.

$$R_{1/2} \approx \frac{4\gamma_{1/2} X_0^{2\gamma_{1/2}-2}}{[\Gamma(2\gamma_{1/2}+1)]^2}$$

$$R_{3/2} \approx \frac{48\, X_0^{\gamma_{1/2}+\gamma_{3/2}-3}}{\Gamma(2\gamma_{1/2}+1)\Gamma(2\gamma_{3/2}+1)} \qquad (66)$$

$$X_0 = 2ZR/a_B$$

The formulae (64),(65),(46),(47) enable us to compare contributions of Q and M to T- and P-odd atomic moments

$$\frac{\langle S|H_{TP}|P\rangle}{\langle S|H_M|P\rangle} \sim \frac{m_e m r_0^2 R_Q A^{2/3}}{R_M} \sim 10^{-2} A^{2/3} \frac{R_Q}{R_M} \qquad (67)$$

m_e, m are electron and proton masses. At $I > 1/2$ the contribution of the MQM is seen to dominate. Only for atoms with heavy spherical nuclei ($A > 200$) the contributions of the Shift moment and MQM become comparable all the more that R_Q has steeper growth with Z than R_M (at $Z = 81$, $R_{1/2} = 7$, $R_{3/2} = 5$, $R_M = 1.8$). As regards nonspherical nuclei, their MQM contribution can be enhanced by an order of magnitude (see sect. 3b).

b) Induced dipole moment of atoms

Note immediately that the nuclear MQM only contributes to EDM in the systems with an unpaired electron angular momentum. The reason is that even with an external electric field $\mathcal{E}$ switched on (it measures EDM) the magnetic field $\mathcal{H}$ of electrons does not arise in an atom with zero angular momentum (it follows from T-invariance that $\vec{\mathcal{H}}$ cannot be proportional to $\vec{\mathcal{E}}$). Consequently, the nuclear MQM does not affect the system state. At the same time, the mixing (65) connected with scalar potential of a nucleus does work in systems with closed electron shells. The latter is of particular importance for molecules where electrons are usually paired.

At first, consider the EDM of a caesium atom. All the necessary calculations have been performed in fact in Ref. [11] (see also [27]) where the atomic EDM induced by the proton EDM has been calculated

$$d_{Cs}^{(M)} = -\frac{4}{15} \frac{M m_e Z^2 \alpha^2 R_M \tau_{6S6P}}{(\nu_{6S}\nu_{6P})^{3/2}} \frac{Ry}{E_{6P}-E_{6S}} \cdot \begin{cases} 1 \\ -\frac{45}{28} \end{cases}$$

$$d_{Cs}^{(Q)} = \frac{16}{9} \frac{Q Z^2 (R_{1/2}+2R_{3/2}) \tau_{6S6P}}{a_B^2 (\nu_{6S}\nu_{6P})^{3/2}} \frac{Ry}{E_{6P}-E_{6S}} \begin{cases} 1 \\ \frac{27}{28} \end{cases} \qquad (68)$$

Here τ_{6S6P} is the radial integral for the E1 amplitude in Bohr radius units. The upper number in the curly bracket corresponds to the atomic total angular momentum $F = I + j = 4$ (and is independent of I), the lower one to $F = 3$. The calculation by the formula (68) with M and Q from Table 1 and with caesium atom parameters from, say, [27] gives (in units of $\eta \cdot 10^{-24}$ e·cm): $d^{(M)} = 2.8$, $d^{(Q)} = -0.23$ at $F = 4$ and $d^{(M)} = -4.5$, $d^{(Q)} = -0.22$ at $F = 3$. Like in the effect induced by the proton intrinsic EDM, the contribution of $d^{(M)}$ is seen to dominate.

From the experimental value $|d_{Cs}| < 3.7 \cdot 10^{-22}$ e·cm obtained for the state with $F = 4$ [10] we find the bound $|\eta| < 130$.

In a similar way the calculations are carried out for the atomic EDM of ^{131}Xe in the metastable state $5p^5\,6s^2\,{}^3P_2$ ($E = 67068$ cm^{-1}) where also the nuclear MQM dominates. The si-

tuation is different in the Xe ground state where the MQM does not work. The EDM here arises mainly due to the interaction of nuclear Schiff moment with the external $5p^6$ shell. The Schiff moment determines also the atomic EDM of thallium, because for stable isothopes ^{203}Tl and ^{205}Tl the MQM is equal to zero. Here the contribution to the EDM is given by a closed $6s^2$ shell as well as by an external 6p electron. The special interest are rare earth atoms due to the presence in their spectra of very close levels of opposite parity. E.g., in samarium there is a metastable level $4f^6(^7F)\,5d\,(^8F)\,6s\;^9F_3$ ($E = 14920.45\ cm^{-1}$) near to which ($\Delta E = 4.62\ cm^{-1}$) there is a level $4f^6\,(^7F)\,6s6p\,(^3P)\;^9G_3$ [32]. This circumstance significantly enhances the EDM of the metastable state. One can get its estimate without difficulty, basing on the calculations for caesium. The effect in samarium arises mainly from $5d$ -6p mixing due to the interaction of electron with nuclear MQM. It follows from the formulae (62)-(64) that the numerical coefficient in the one-particle matrix element (61) in this case is 5÷10 times less than for a s-p transition. Moreover, complex many-body states with number of simple components up to 10 (but not the one-particle ones) are mixing here in fact. And this makes the effect smaller by another order of magnitude. Thus, the EDM of the metastable state of samarium exceed that of caesium by two orders of magnitude (and not by four orders, as one can suspect comparing energy intervals). The more accurate calculation using the wave functions of mixing states from [32] confirms this estimate.

The near level of opposite parity $2P$ enhances the EDM in the metastable 2s-state of deuterium: $d_D \sim 0.5\cdot10^{-22}\eta\,e\cdot cm$. The principal contribution here is produced by magnetic quadrupole and direct contribution of the deuteron EDM connected with the Shiff theorem violation caused by hyperfine interaction. The inconvenience of experiment with deuterium is that the electric field causes the quenching of 2S-level.

The calculated EDM of atoms are presented in Table 2.

c) Induced dipole moment of molecules.

In the papers [28,33,34] it was shown that due to the small interval between rotational levels of opposite parity the effects of T- and P-invariance violation in polar molecules are considerably enhanced. At first, consider the diatomic molecules with paired electron angular momentum. As we have already seen, the nuclear MQM does not work here, and the molecular EDM in the stationary state arises due to Shiff moment.

In order to explain how one can obtain the bound on the T- and P-odd interaction constant from the experimental data on the search for the T-invariance violation in the molecule TlF [5-7], we consider a simple model of the electronic structure of this molecule. We suppose that the outer electron of the Tl atom goes to the F atom. The distance between nuclei is $r_e = 3.92\,a_B$ [35]. The Tl^+ ion is then in the electric field $\mathcal{E} = e/r_e^2$, which polarizes the outer shell $6S^2$. Therefore, one-particle orbitals become a mixture of 6s- and 6p-states:

$$|\omega\rangle = |6S,\omega\rangle + \beta\left[-\frac{2\omega}{\sqrt{3}}|6P_{3/2},\omega\rangle + \sqrt{\frac{2}{3}}|6P_{3/2},\omega\rangle\right]$$

$$\beta = \frac{2}{\sqrt{3}}\,\frac{Ry}{E_{6S}-E_{6P}}\,\frac{r_{6S6P}}{r_e^2} = 0.27 \qquad (69)$$

Here r_{6S6P} is the radial integral and E_{6S}, E_{6P} are the energies for Tl^+. The quantities r_{6S6P}, r_e are expressed in units of a_B, $\omega = \pm 1/2$ is the projection of one-electron angular momentum on the molecular axis. With the aid of formulae (69) and (65) we find the effective Hamiltonian of the T- and P-odd interaction of the spin of the Tl nucleus with the molecular axis $\vec{N}$:

$$\frac{H_{eff}}{Ry} = \frac{32}{3\sqrt{3}}\,\beta\,\frac{Z_i^2 Z^2 (R_{1/2}+2R_{3/2})}{(\gamma_{6S}\,\gamma_{6P})^{3/2}}\,\frac{\vec{Q}\vec{N}}{e a_B^3} = 1.1\cdot10^5\,\frac{\vec{Q}\vec{N}}{e a_B^3} \qquad (70)$$

The effective charge of Tl^+ is $Z_i = 2$, $\gamma_{6s} = 1.63$, $\gamma_{6p} = 2.15$ ($E = -z_i^2 Ry/\nu^2$), $Z_{6p6s} = 2.3$. The more accurate calculation [8] leads to the result 2.5 times less than (70). Taking into account this circumstance and using the value of Q_{Tl} from Table 1, we obtain:

$$H_{eff}(TlF) = Ry \cdot \mathcal{K}_{Tl} \left(\frac{\vec{I}}{I}\right)_{Tl} \vec{N}, \quad \mathcal{K}_{Tl} = -0.6 \cdot 10^{-17} \eta \qquad (71)$$

The index Tl means that we have in mind the interaction of the spin of Tl nucleus with the molecular axis. The best of the experimental bounds on the constant $\mathcal{K}_{Tl}$ is [7]:

$$\mathcal{K}_{Tl}\, Ry = 2\pi\hbar\, (8 \pm 12) \cdot 10^{-3}\ Hz \qquad (72)$$

It follows from (71) and (72) that

$$\eta = -0.4 \pm 0.6 \qquad (73)$$

The estimate (71) is valid for the other compounds of Tl with halogenes since they have analogous electronic structure. In the TlI molecule, interaction of the iodine nucleus spin with the molecular axis becomes also of importance. We estimate its value starting from the calculation [8] for the TlF molecule and taking into account the regular factor of growth with Z from fluorine to iodine: $Z^2 (R_{1/2} + R_{3/2})$ (see (65)).

$$H_{eff} = -0.16 \cdot 10^5 Ry \frac{\vec{Q}\vec{N}}{e a_B^3} = Ry\, \mathcal{K}_I \left(\frac{\vec{I}}{I}\right)_I \vec{N}, \quad \mathcal{K}_I = 0.15 \cdot 10^{-17} \eta \qquad (74)$$

Comparing (74) with (71) we see that the contribution of the Tl nucleus still dominates perhaps. About the same value as $\mathcal{K}_{Tl}$ in the molecule TlF (Cl,Br,I) has $\mathcal{K}_{B_i}$ in the molecule BiF (Cl, Br, I). And probably, $\mathcal{K}_{Np}$ in the molecule NpF is 4-6 times larger due to larger Z and Q of the neptunium nucleus (if such a molecule exists and has sufficiently simple electronic structure).

And at last, on the molecule CsI which seems to be very convenient from the experimental point of view. Here also in

the first approximation there is one extra electron on the iodine atom and by its electronic wave-function near I it resembles TlI. Therefore, one should expect that $\mathcal{K}_I$ has about the same value as in the TlI molecule. The same order of magnitude has also $\mathcal{K}_{Cs}$. The largest of two values of the constants $\mathcal{K}$ for the molecules considered are presented in the Table 3. Emphasize that these values are in fact estimates accurate up to a factor of 2-3.

Calculate now the T- and P-odd molecular EDM in the stationary rotational state. The experiment is carried out in a magnetic field, breaking the hyperfine structure due to the interaction of nuclear magnetic moment with rotational one. Therefore one can write the molecular wave function as a product

$$|\Psi\rangle = |I, I_z\rangle |L, L_z\rangle \qquad (75)$$

L denotes rotational angular momentum of the molecule. The EDM in the state (75) arises due to the T- and P-odd mixing of rotational states of opposite parity by the interaction $H_{eff} = \mathcal{K} Ry\, \vec{N}\vec{I}/I$.

$$d_z = \sum_{L'L'_z} 2 \frac{\langle I I_z | \langle L L_z | H_{eff} | L' L'_z \rangle | I I'_z \rangle \langle I I'_z | \langle L' L'_z | \mathcal{D}_{mol} N_z | L_z \rangle | I I_z \rangle}{E_L - E_{L'}} =$$

(76)

$$= 2\mathcal{K} Ry\, \mathcal{D}_{Mol} \frac{I_z}{I} \sum_{L'} \frac{|\langle L L_z | N_z | L' L_z \rangle|^2}{E_L - E_{L'}} =$$

$$= \frac{\mathcal{K} Ry}{B} \mathcal{D}_{Mol} \frac{I_z}{I} \frac{L(L+1) - 3L_z^2}{L(L+1)(2L-1)(2L+3)}$$

Here $\mathcal{D}_{Mol}$ denotes the dipole moment of a polar molecule in its rest frame (see [35,36]), $E_L = B L(L+1)$. The formula

(76) is valid at not too strong electric fields: $\mathcal{D}_{mol}\mathcal{E} \ll B\cdot 2(L+1)$. In an arbitrary field the Stark shift of energy levels can be found by means of plots of $\langle N_z\rangle$ from the Ref. [37]. The EDM is maximal at $L=0$, $I_z=I$:

$$d = -\frac{\varkappa\, Ry}{3B}\,\mathcal{D}_{mol} \qquad (77)$$

The numerical values of d for the molecules considered are given in Table 3. Due to smaller rotational interval the EDM of the iodine compounds exceeds those of fluorine ones. However, at the electric field $\mathcal{E} \sim 5 \div 10$ kV/cm this advantage disappears because the molecular polarization degree does not practically increase further.

Pass now to the molecules with an unpaired electron angular momentum. The effect of nuclear MQM dominates here. Take as an example the ^{201}HgF molecule. The electron state of this molecule is $^2\Sigma$. The electron spin in such state, as known, can be regarded as being uncoupled from the molecular axis. Therefore, only the orbital electron wave function need to be considered in the rest frame of the molecule. We find this wave function assuming that one outer electron of mercury atom goes to F. The wave function of the remaining electron has the form (cf. (69))

$$|\Sigma\rangle = |6S\rangle + \beta|6P\rangle, \qquad \beta = \frac{2}{\sqrt{3}}\frac{Ry}{E_{6S}-E_{6P}}\,\frac{\gamma_{6S6P}}{\gamma_e^2} \approx 0.27 \qquad (78)$$

Now, considering the expression in the brackets in the formula (61) as an operator, with the aid of (78) we find an effective Hamiltonian

$$\frac{H_{eff}}{Ry} = \frac{Mm_e}{e a_B}\,\frac{Z_i^2 Z^2\alpha^2 R_M}{2\sqrt{\gamma_{6S}^3\gamma_{6P}^3}}\,\frac{t_{mK}\delta_e}{I(2I-1)}\langle\Sigma|\delta_{em}n_K + \delta_{eK}n_m - 2n_e n_K n_m|\Sigma\rangle =$$

(79)

$$= \frac{2\sqrt{3}\beta}{5}\,\frac{Mm_e}{e a_B}\,\frac{Z_i^2 Z^2\alpha^2 R_M}{\sqrt{\gamma_{6S}^3\gamma_{6P}^3}}\,\frac{t_{mK}\delta_m N_K}{I(2I-1)}$$

Deriving (79), we take into account the relation

$$\langle\Sigma|\delta_{em}n_K + \delta_{eK}n_m - 2n_e n_K n_m|\Sigma\rangle = \frac{2\sqrt{3}\beta}{5}\left[\delta_{em}N_K + \delta_{eK}N_m - \tfrac{2}{3}\delta_{mK}N_e\right]$$

Due to the magnetic interaction between the electron spin and nuclear one the stationary state has a fixed F, $\vec F = \vec I + \vec S$. Using the formulae

$$\langle F|t_{mK}\delta_m|F\rangle = A F_K,$$

$$A = \frac{x^2 + \frac{4}{3}I(I+1)\left(x-\frac{3}{4}\right)}{F(F+1)}, \qquad x = F(F+1) - I(I+1) - 3/4, \qquad (80)$$

we pass from (79) to the effective Hamiltonian

$$H_{eff} = Ry\,\varkappa\,\frac{\vec F\vec N}{F} \qquad (81)$$

$$\varkappa = \frac{4\beta}{5\sqrt{3}}\,\frac{Mm_e}{e a_B}\,\frac{Z_i^2 Z^2\alpha^2 R_M}{\sqrt{\gamma_{6S}^3\gamma_{6P}^3}}\begin{cases} 1 & F = I + 1/2 \\ -\dfrac{(I+1)(I+3/2)}{I(I+1/2)} & F = I - 1/2 \end{cases}$$

For Hg^+ the parameters Z_i, γ_{6S}, γ_{6P}, γ_{6P6S} are practically the same as for Tl^+ (see the calculation of TlF). We assume as for the case of TlF that an answer (81) is overestimated by a factor of 2.5. As a result we find

$$\varkappa_{Hg} = -3\cdot 10^{-17}\,\eta\cdot\begin{cases} -0.4 & F = 2 \\ 1 & F = 1 \end{cases} \qquad (82)$$

The result of similar calculations for molecules BaF and BaI are given in Table 4. Due to large nuclear MQM of ^{161}Dy and ^{237}Np (see Table 1) it can be expected that $\mathcal{K}$ for DyF and NpO is about 20 times larger than that for HgF, of course, if these molecules have sufficiently simple electronic structure.

Now we calculate T- and P-odd dipole moment of molecules with an unpaired electron spin in a definite rotational state. We suppose that in the first approximation $\vec{F}$ is uncoupled from the rotation, $|\Psi\rangle = |F, F_z\rangle\,|l, l_z\rangle$. Then analogously to (76) we obtain

$$d_z = \frac{\mathcal{K} Ry}{B} \mathcal{D}_{Mol}\ \frac{F_z}{F}\ \frac{l(l+1) - 3l_z^2}{l(l+1)(2l-1)(2l+3)} \qquad (83)$$

At $l=0$, $F_z = F$

$$d = -\frac{\mathcal{K} Ry}{3B} \mathcal{D}_{Mol}$$

The numerical values of d are given in Table 4. For molecules BiO, BiS due to the strong coupling of the electron spin with the molecular axis the above calculation is not applicable literally. Nevertheless for these molecules one can expect for the EDM the same or even greater value than for HgF ($d \sim 10^{-19}\,\eta\cdot e\cdot cm$). The molecules LaO, LaS can be also suitable.

5. Conclusion

The regular enhancement of T- and P-odd multipoles in atomic nuclei drastically increases the actual physical value of experiment on the search for T-invariance violation in atoms and molecules. While the gap in experimental bounds on nucleon EDM (1) and (2) amounts to three orders of magnitude, the difference in corresponding bounds on the superweak interaction constant η is only an order of magnitude weaker (cf. (1) and (6b), (73) and (20a)).

Moreover, just going from TlF to other compounds without increasing absolute accuracy of the molecular experiment, the advance by one or two orders of magnitude might be achieved. The dipole moment values of dysprosium and neptunium

compounds expected from KM model (see Table 4) are close to the sensitivity of experiments on the search for the neutron EDM. Even if diatomic molecules of dysprosium and neptunium are difficult to synthesize one might think about their more complex compounds among which there are some volatile as well (see [38]). Remind that dysprosium has a stable isotope and neptunium has almost stable isotope where T-odd moments are additionally enhanced by about an order of magnitude due to the presence of close levels of opposite parity in their nuclei.

As regards the atomic experiments, the efficiency here might be increased by about two orders of magnitude by going to metastable states of rare-earths, where anomalously small energy intervals between opposite parity levels exist. On the other hand, the obvious experimental advantages of the usual atomic xenon in the ground state could overweight with odds the suppression of the effect taking place in it in comparison, say, with atomic caesium. Moreover, the experiment could be performed with liquid xenon. In this connection, we would like to drow once more attention to the possibility of the search for the T-invariance violation by means of NMR in the liquid phase. This possibility was discussed in detail earlier in Ref. [39].

Of particular interest might be the experiments of NMR type in ferroelectric, where the effective electric field acting on nucleus is not much smaller than the atomic one. In other words, here the enhancement of the effect of the same kind as in the diatomic polar molecule occurs.

And at last, in experiments with superfluid ^{3}He in the polarized A_1 -phase one might expect that the EDM of ^{3}He nucleus would be measured at the level $\sim 10^{-27}$ e.cm [40]. From Table 1, this number is seen to exceed by two orders of magnitude only the KM model prediction.

Therefore, atomic and molecular experiments undoubtedly still have unexploited possibilities for the significant advance in exploring the nature of the CP-invariance violation.

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A P P E N D I X

We list for reference the quasiclassical formulae used for calculations of the EDM of ground and metastable states of xenon and thallium atom. In the ground state of xenon the electron angular momentum is zero and the EDM arises due to interaction of electrons with the nuclear Schiff moment. Assuming that the principal contribution is given by the $5p^6$ shell, we find

$$d_{Xe} = \frac{32}{9} Q \frac{Z^2}{a_B^2} (R_{1/2} + 2R_{3/2}) \sum_{ns} \frac{\zeta_{5p\,ns}}{\sqrt{\nu_{5p}^3 \nu_{ns}^3}} \frac{Ry}{E_{ns} - E_{5p}}$$

For the numerical estimate we have taken $E_{ns} - E_{5p} \approx Ry$, $\nu_{5p} \simeq \nu_{ns} \simeq 1$, $\zeta_{5p\,ns} \simeq 1$. These numbers are in a reasonable correspondence with known polarizability of a xenon atom. In the metastable state $^3P_2$ ($E = 67068\ cm^{-1}$) the principal contribution to the atomic EDM is given by the nuclear MQM if nuclear angular momentum $I > 1/2$. Therefore consider the ^{131}Xe isotope with $I = 3/2$. The wave function of the $^3P_2$ state has the form

$$|^3P_2, J_z = 2\rangle = |\overline{5P}_{3/2}, j_z = 3/2\rangle |6S_{1/2}, j_z = 1/2\rangle,$$

where $|\overline{5P}_{3/2}\rangle$ is the wavefunction of the $5p^6$ shell with a hole in $5P_{3/2}$ state. The principal contribution to the EDM is given by mixing with $|\overline{5P}_{3/2}, j_z = 3/2\rangle |6P_{3/2}\rangle$ states. The energies of these states are in the range 78000- $80000\ cm^{-1}$.

In the simplest case, when the total angular momentum is maximal ($F = I + J = 7/2$) the answer for the EDM has the same form as for the caesium

$$d_{Xe} = -\frac{4}{15} \frac{M m_e Z^2 \alpha^2 R_M}{(\nu_{6s}\, \nu_{6p})^{3/2}} \zeta_{6s6p} \frac{Ry}{E_{6p} - E_{6s}}$$

The numerical value is obtained at $\nu_{6s} = 1.9$, $\nu_{6p} = 2.5$,

The experiment on the measurement of the EDM of the metastable state $3p_2$ had the same sensitivity as that with caesium but was carried out, as far as we know, only for the even isotope of xenon. Therefore, the bound on the constant η cannot be derived from it. The angular momentum of nuclei ^{203}Tl and ^{205}Tl is equal to $I = 1/2$, and only the Shiff moment of the nucleus works here. In the ground state of thallium at $F = I + j = 1$ the EDM is equal to

$$d_{Tl} = \frac{16}{9} Q \frac{Z^2}{a_B^2} \left\{ \sum_{ns} \frac{\gamma_{6p_{1/2}} ns \; R_{1/2}}{(\nu_{ns}\, \nu_{6p_{1/2}})^{3/2}} \frac{Ry}{E_{ns} - E_{6p_{1/2}}} + \right.$$

$$\left. + 2 \sum_{np} \frac{\gamma_{np6s} \, (R_{1/2} + 2R_{3/2})}{(\nu_{6s}\, \nu_{np})^{3/2}} \frac{Ry}{E_{np} - E_{6s}} \right\}$$

The sums in this formula are saturated practically by $6p - 6s$, $7s$ transitions. The necessary values for the parameters ν, E, γ can be found, e.g., in Ref. [27].

	Nucleus	Unpaired nucleon	$\frac{d}{\eta}(e\cdot cm)\cdot 10^{21}$	$\frac{Q}{\eta}(e\,fm^3)\cdot 10^{8}$	$\frac{M}{\eta}(\frac{e}{m_p}\,fm)\cdot 10^{7}$
spherical nuclei	$^{127}I_{53}$	$p, d_{5/2}$	1.2	-1.4	-1.4
	$^{131}Xe_{54}$	$n, d_{3/2}$	0.5	~0.2	-0.5
	$^{133}Cs_{55}$	$p, g_{7/2}$	-0.9	3.0	1.7
	$^{135,137}Ba_{56}$	$n, d_{3/2}$	0.5	~0.2	-0.5
	$^{147,149}Sm_{62}$	$n, f_{7/2}$	-0.8	~0.2	2.3
	$^{201}Hg_{80}$	$n, p_{3/2}$	-0.8	~0.2	0.8
	$^{203,205}Tl_{81}$	$p, s_{1/2}$	1.2	-2	-
	$^{209}Bi_{83}$	$p, h_{9/2}$	-1.0	3.8	2.3
deformed nuclei	$^{161}D_{66}$	$n, 5/2^+$	7	~1	27
	$^{237}Np_{93}$	$p, 5/2^+$	1	4	20
light nuclei	$^{2}H_1$		2	0	1
	$^{3}He_2$		1	~0.1	-
	Neutron		$5\cdot 10^{-3}$		

Table 1

Electric dipole, Shiff and magnetic quadrupole moments of the nuclei. Parameter η is a coefficient in the Hamiltonian of P- and T-odd interaction (19). Presented value of neutron EDM is obtained from (6b) by means of division by η_n (20a).

Atom	^{133}Cs		^{131}Xe		$^{203,205}Tl$	$^{147,149}Sm$
State	F = 3	F = 4	ground state	$3p_{\frac{1}{2}}$, $F=\frac{1}{2}$	F = 1	E = 14929 cm^{-1}
$\frac{d}{\eta}\cdot 10^{24}$ (e·cm)	- 4.7	2.6	0.01	-0.7	0.3	200

Table 2

Atomic E D M

	TlF	TlI	BiF	BiI	NpF	NpI	CsF	CsI
$\left\|\frac{x}{\eta}\right\|\cdot 10^{17}$	0,6		0,6		3		0,15	
$\left\|\frac{d}{\eta}\right\|\cdot 10^{20}$ (e·cm)	0,9	7	0,9	7	4	30	0,5	5

Table 3

Constants of P- and T-odd interaction of nuclear spin with molecular axis (see (71)) and EDM of molecular ground state

	BaF	BaI	HgF	HgI	DyF	DyI	NpO	NpS
$\left\|\frac{x}{\eta}\right\|\cdot 10^{17}$	0,6		3		~50		~50	
$\left\|\frac{d}{\eta}\right\|\cdot 10^{20}$ (e·cm)	1,5	15	4	30	~70	~500	~70	~150

Table 4

Constants of P- and T-odd interaction of angular momentum $\vec{F} = \vec{I} + \vec{S}$ with axis (see (81)) and EDM of the molecules at F = I - S, L = 0.

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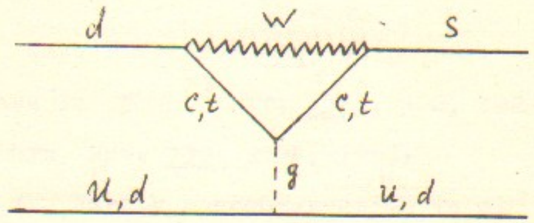

Fig 1

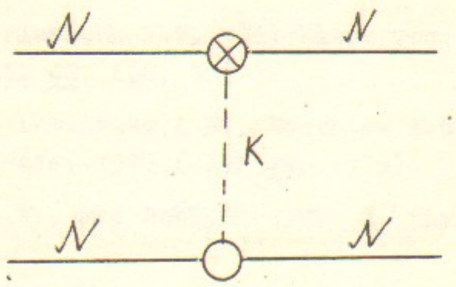

Fig 2

О.П.Сушков, В.В.Фламбаум, И.Б.Хриплович

К ВОЗМОЖНОСТИ ИССЛЕДОВАНИЯ P- и T-НЕЧЕТНЫХ ЯДЕРНЫХ СИЛ В АТОМНЫХ И МОЛЕКУЛЯРНЫХ ЭКСПЕРИМЕНТАХ

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