# Possibility of investigating *P*- and *T*-odd nuclear forces in atomic and molecular experiments

O. P. Sushkov, V. V. Flambaum, and I. B. Khriplovich

*Nuclear Physics Institute, Siberian Division, USSR Academy of Sciences*
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The *P*- and *T*-odd nucleon-nucleon potentials are found in the Kobayashi-Maskawa scheme. Analytic expressions for *T*-odd nuclear multipoles are obtained in the shell model. The electric dipole moments of the nuclei exceed that of the neutron by two to three orders of magnitude. The electric dipole moments are calculated for a number of atoms and molecules. The feasibility of experimental detection of *T*-invariance violation is discussed.

## 1. INTRODUCTION

Although many years have already elapsed since the discovery[1] of *CP* nonconservation, neutral-kaon decays remain as before the only physical phenomena in which this effect was observed. Hence the great interest in searches for the electric dipole moments (EDM) of elementary particles, one more possible manifestation of possible *CP* nonconservation.[2] Continuing prolonged experiments by many groups (see, e.g., the review by Ramsay[3]) led to constraints on the EDM of the neutron; the most stringent of them is[4]:

$$|d_n/e|<4\cdot10^{-25}\,\text{cm}. \tag{1}$$

These constraints permitted a drastic decrease in the number of possible *CP*-nonconservation models.

The constraint considered to be the best for the proton EDM (we shall return to the question of its reliability below) was obtained in experiments with the TlF molecule.[5–7] According to the latest calculations, it states that[8]

$$d_p/e=(2{,}3\pm3{,}4)\cdot10^{-21}\,\text{cm}. \tag{2}$$

The constraint that follows from experiments with atomic cesium[9,10] takes the form[11]

$$|d_p/e|<5{,}5\cdot10^{-19}\,\text{cm}. \tag{3}$$

Both constraints (2) and (3) were obtained under the assumption that the EDM of the thallium and cesium atoms investigated in the experiments are due to the dipole moment of the valence proton.

It is difficult, however, to imagine a situation in which a difference of several orders of magnitude can exist between the proton and the neutron, two strongly interacting particles that are virtually transformed easily into each other (e.g., $n\leftrightarrow p\pi^-$, $p\leftrightarrow n\pi^+$). An impression is therefore gained that measurements of EDM of atoms are of no particular interest in elementary-particle physics.

This is not the case, however from our point of view. It is shown in the present paper that the dipole moment induced by *T*- and *P*-odd nucleon-nucleon interactions can exceed the nucleon EDM by more than 100 times. Additional enhancement of the EDM of a nucleus can result from the anomalous proximity of nuclear levels of opposite parity. The last circumstance was first noted in Ref. 12 and discussed in detail quite recently in Refs. 8 and 13. It seems to us, however, that this additional enhancement factor can hardly exceed 10 in stable nuclei.

The indicated nuclear EDM enhancement shortens substantially the gap between the experimental data obtained on *CP* nonconservation in the already performed spectroscopic and neutron experiments. The possibilities of further progress in molecular and atomic experiments is also discussed in the present paper.

## 2. *P*- AND *T*-ODD INTERNUCLEON POTENTIAL IN THE KOBAYASHI-MASKAWA MODEL

The success of the renormalizable theory of electromagnetic and weak interactions makes it quite natural to attempt to describe *CP* nonconservation within the framework of this very same approach. Two schemes of this type are being most intensively discussed (we disregard here models based on grand unification theories or on supersymmetries). In one of them the *CP* nonconservation arises in the Higgs sector of the theory,[14,15] and in the other, in the fermion sector.[16] As for the most popular variant of the model of the first type, proposed by Weinberg,[15] the neutron EDM[17,18] that follows from it

$$d_n/e\approx-9\cdot10^{-25}\ \text{cm} \tag{4}$$

contradicts even formally the constraint (1). There are also indications that this model contradicts the *CP* nonconservation parameters in $K_L\to2\pi$ decays.[19,20] We consider therefore a *P*- and *T*-odd potential in a *CP*-nonconservation scheme of another type—the Kobayashi-Maskawa (KM) model.[16] It was shown independently in Refs. 18 and 21 that the main contribution to the neutron EDM is made by the effective quark-quark interaction operator

$$\hat{H}=i\frac{G_1}{\sqrt{2}}\bar{s}\gamma_\mu(1+\gamma_5)\lambda^a d\sum_{q=u,d}\bar{q}\gamma_\mu\lambda^a q,$$
$$G_1=Gs_1s_2s_3c_2\sin\delta\frac{\alpha_s\Delta}{12\pi}\ln\frac{m_t^2}{m_c^2}, \tag{5}$$

which is described by the "penguin" diagram[22] of Fig. 1 (the dashed line in it represents a gluon). Here $G=10^{-5}m_p^{-2}$ is the Fermi constant of the weak interaction; for the KM matrix and its parameters $\delta, s_i$, $c_i$ we use Okun's notation,[23] assuming here $s_2s_3c_2\sin\delta\simeq10^{-3}$. For the strong-interac-

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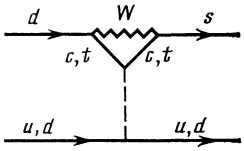


FIG. 1.

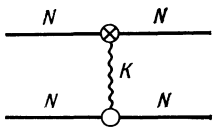


FIG. 2.

tion constant we assume the value $\alpha_s = 0.2$. The correction factor $\Delta$ that takes strong interactions at short distances into account is equal to 1.3 if gluons with virtuality from $m_t$ to $m_c$ are considered; if, however, we go to a lower value, say 0.2 GeV, we have $\Delta = 2.5$. This operator is special because it contains right-hand currents whose matrix elements are noticeably enhanced (see Ref. 22). Furthermore, the mutual cancellation of the contributions of the $t$ and $c$ quarks in the limit $m_t = m_c$ is ensured here not by the usual factor $(m_t^2 - m_c^2)/m_w^2 \sim 0.1$, but by $\ln(m_t^2/m_c^2) \sim 6$.

The dipole moment of the neutron in the KM model at $\Delta = 1.3$ is[18]

$$d_n/e = 2\cdot 10^{-32}\ \text{cm}, \tag{6a}$$

and at $\Delta = 2.5$ we have

$$d_n/e = 4\cdot 10^{-32}\ \text{cm}. \tag{6b}$$

This is precisely the value of $d_n$ that we shall use hereafter. The larger value $d_n/e \sim 10^{-30}$ cm obtained in Ref. 21 is most likely an overestimate.[24,25]

When using the operator (5) to construct the $P$- and $T$-odd internuclear potentials we confine ourselves to pole diagrams; this, at any rate, enables us to avoid small geometric quantities of the type $1/\pi^2$ which stem from the loops. The simplest diagram of this type is shown in Fig. 2: the $CP$-odd vertex, marked $\otimes$, should be pseudoscalar, for it is precisely in this case that the matrix element of the operator (5) is enhanced by the right-hand currents. The $CP$-odd vertex $\circ$ should then be a scalar, and $s$ wavelike.

The standard factorization technique allows us to reduce the pseudoscalar part of the matrix element $\langle pK^-|\hat{H}|n\rangle$ to the form

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

Here $f_K =$ MeV is the $K\to\mu\nu$ decay constant, $g_a = 1.15$ is the axial-current renormalization constant, and for the quark current masses $m_s$, $m_d$, and $m_u$ we assume the values 150, 7, and 4 MeV, respectively.

The calculation of the matrix element $\langle NK^0|\hat{H}|N\rangle$, $N = p$, $n$ reduces in the same technique to calculation of $\langle \bar{N}|\bar{d}\gamma_5 d|N\rangle$. The nucleon matrix element of the divergence of the isovector axial current

$$j_{\mu 5}^{(1)} = {}^1/_2(\bar{u}\gamma_\mu\gamma_5 u - \bar{d}\gamma_\mu\gamma_5 d)$$

leads to the equality

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

where

$$\tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

is the isotopic-spin operator. From isotopic-invariance considerations it follows that the matrix element

$$\langle N|\bar{u}\gamma_5 u + \bar{d}\gamma_5 d|N\rangle$$

contains no pion pole, so that in the chiral limit we have

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

From (8) and (9) we obtain

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

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

The scalar vertex in Fig. 2 can be expressed in terms of the $s$-wave amplitudes of the hyperon nonleptonic decays. Using the octet-dominance hypothesis, we write down the $s$-wave $CP$-odd baryon ($B$) and pseudoscalar ($P$) octet interaction amplitude in the form (see, e.g., Ref. 23)

$$A_3[(PS\bar{B}B) - (SP\bar{B}B)] + A_4[(PSB\bar{B}) - (SPB\bar{B})] + A_7[(S\bar{B})(BP) - (SB)(\bar{B}P)]. \tag{12}$$

The spurion $S \sim \lambda_6$ is here the sixth component of the octet, and the parentheses enclose matrix-product traces. The coefficients $A_{3,4,7}$ are expressed in terms of the $s$-wave amplitudes of the nonleptonic hyperon decays (we use for these amplitudes the phase system adopted in Ref. 22) as follows:

$$A_3 = -\sqrt{2}A(\Sigma_0^+) = -2.1, \quad A_7 = A(\Sigma_+^+) = 0.06,$$
$$A_4 = -\sqrt{\frac{3}{2}}A(\Lambda_-^0) - \frac{1}{\sqrt{2}}A(\Sigma_0^+) = 0.77. \tag{13}$$

As a result, the effective Hamiltonian of the $s$-wave $CP$-even kaon-nucleon interaction takes the form

$$\hat{H}_w = -iGm_\pi^2\{A_3(\bar{p}p)(K^0-\bar{K}^0) + (A_3-A_4+A_7)(\bar{n}n)(K^0-\bar{K}^0) + (A_4-A_7)[(\bar{n}p)K^- - (\bar{p}n)K^+]\}. \tag{14}$$

We note that since the squared momenta of the pion in hyperon decay ($q^2 = m_\pi^2$) and of the kaon in intranuclear exchange ($|q|^2 \sim m_\pi^2$) are small when measured in hadron scale, the coefficients $A_{3,4,7}$ in (14) are close to the values (13) obtained from nonleptonic decays.

Using Eqs. (7) and (11) (and their Hermitian adjoints), as well as (14), we arrive at the following $CP$-odd nucleon-nucleon interaction Hamiltonian

$$\frac{G}{\sqrt{2}}\eta_0\frac{m_\pi^2}{m_\pi^2-q^2}\{i[(\bar{p}\gamma_5 p) - (\bar{n}\gamma_5 n)][(\bar{p}p) + 1.34(\bar{n}n)] - 0.34i[(\bar{p}\gamma_5 n)(\bar{n}p) + (\bar{n}\gamma_5 p)(\bar{p}n)]\}. \tag{15}$$

In this expression

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

In the derivation of (15) we took it into account that the characteristic momentum transfers in the nucleus are much smaller than $m_K$, so that the $K$-meson propagator is $(q^2 - m_K^2)^{-1} \approx -m_K^{-2}$.

After a Fierz transformation, the last term in (15), due to charged-kaon exchange, reduces in the momentum representation and in the nonrelativistic approximation to

$$-\frac{G}{\sqrt{2}} \frac{\eta_0}{2m} 0.17 [\boldsymbol{\sigma}_p \times \boldsymbol{\sigma}_n] (\mathbf{p}_{fn} + \mathbf{p}_{in} - \mathbf{p}_{fp} - \mathbf{p}_{ip}). \quad (17)$$

Here $\boldsymbol{\sigma}_p$ and $\boldsymbol{\sigma}_n$ are the proton and neutron spin operators, while $\mathbf{p}_i$ and $\mathbf{p}_f$ are the initial and final momenta of the corresponding particles. In this and following formulas we omit for simplicity the factor $m_\pi^2/(m_\pi^2 - q^2)$, which makes the interaction nonlocal in coordinate space. The interaction (17) does not work in either an ordinary nucleus, in which the angular momenta of all nucleons but the outer one are compensated, nor, e.g., in the deuteron, where the total nuclear spin is specified and is not altered by the dipole-moment operator; this interaction will therefore be disregarded hereafter. It is curious that in the case of a $P$-odd but $T$-even nucleon-nucleon interaction the exchange term with the analogous Lorentz structure turns out to be quite substantial.

In none of the other possible mechanisms that lead to the appearance of $P$- and $T$-odd nuclear forces in the Kobayashi-Maskawa model were we able to observe any mechanism capable of competing successfully with $K$-meson pole exchange. We shall confine ourselves hereafter to just this interaction, which we write in the form

$$\frac{G}{\sqrt{2}} \eta_0 i [(\bar{p}\gamma_5 p) - (\bar{n}\gamma_5 n)][(\bar{p}p) + 1{,}34(\bar{n}n)], \quad (18)$$

and leave out of (15) the last, exchange term.

In a heavy nucleus, the $P$- and $T$-odd interaction of a nonrelativistic nucleon with the core is described by the following effective Hamiltonian:

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

where $\boldsymbol{\sigma}$ is the spin of this nucleon and $\rho$ is the density of the core neutrons and protons. This phenomenological expression for the interaction is not connected in essence with any concrete $CP$-nonconservation scheme at the elementary-particle level, and is thus quit general. In the Kobayashi-Maskawa model, which is of primary interest to us,

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

where $Z$ is the charge of the nucleus and $A$ is the atomic number. Numerically we have at $Z \gtrsim 40$

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

It must be borne in mind, however, that the Kobayashi-Maskawa model predicts most likely the lowest values for $T$-odd multipole moments.

## 3. NUCLEAR ELECTRIC DIPOLE AND MAGNETIC QUADRUPOLE MOMENTS DUE TO $P$- and $T$-ODD NUCLEON-NUCLEON INTERACTIONS

The simplest $P$- and $T$-odd characteristic of a nucleus is the electric dipole moment

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

where $\delta\rho$ is the correction to the charge density necessitated by the $P$- or $T$-odd interaction. If, however, a neutral atom or molecule is regarded as a system of pointlike particles with Coulomb interaction then, even though the nucleus has an EDM, the total dipole moment of the system is zero in accordance with Schiff's well known theorem.[26] (A detailed analysis of a number of problems connected with this theorem can be found, e.g., in Khriplovich's book[27].) It was noted in Ref. 26, however, that this hindrance is lifted, in particular, when the finite dimensions of the nucleus are taken into account. It was shown subsequently[28] that it is precisely this effect which is the main cause of violation of Schiff's theorem in heavy atoms and molecules. The Schiff hindrance reduces to the fact that the $P$- and $T$-odd potentials of the nucleus must be written in the form

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

where $\rho_0(r)$ is the spherically symmetric charge density of the nucleus, normalized by the condition $\int d^3 r \rho_0(\mathbf{r}) = Z$. The second term in (22) ensures, in accord with Schiff's theorem, the vanishing of the dipole term of the expansion of the potential outside the nucleus. The total EDM of the atom or molecule is the electron-shell dipole moment induced by the potential (22).

In the calculation of the EDM of the nucleus, or of the potential (22), it is necessary to take into acount the motion of the nuclear core besides the motion of the outer nuclei. It is known that the large mass core, even in heavy nuclei, is compensated for by the large charge. Let $\delta\rho_v$ be the $T$- or $P$-odd correction to the probability density, due to the outer (valence) nucleon of the nucleus. The total charge-density correction that enters in (21) and (22) is then

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

where $q = 0$ and 1 respectively for the neutron and proton, and $\langle r \rangle$ is the contribution to the dipole moment of the nucleus, necessitated by the unpaired nucleon:

$$\langle \mathbf{r} \rangle = \int \delta\rho_v(\mathbf{r}) \mathbf{r} d^3 r. \quad (24)$$

The second term in (23) takes into account the fact that when the outer nucleon moves the core is shifted relative to the mass center ($\mathbf{r}_C \approx -\mathbf{r}/A$), and this alters the charge density $\rho_0(\mathbf{r} - \mathbf{r}_C) - \rho_0(\mathbf{r}) \approx \mathbf{r}\nabla\rho_0(r)/A$. With the recoil effect (23) taken into account, the EDM of the nucleus takes, as expected, the form

$$\mathbf{d}=d(\mathbf{I}/I)=e(q-Z/A)\langle\mathbf{r}\rangle. \tag{25}$$

With the aid of (23) it is easy to verify that the recoil effects in the two terms of Eq. (22) for $\delta\varphi$ cancel out exactly:

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

Thus, $\delta\varphi$ assumes the form that would be obtained without taking any account of the recoil. The potential (26) can be expanded in powers of $R^{-1}$:

$$\delta\varphi(\mathbf{R})=eq\left[-\frac{1}{6}\int\delta\rho_V r_n r_m r_l\,d^3r+\frac{1}{2}\langle r_m\rangle\int\frac{\rho_0}{Z}r_n r_l\,d^3r\right]\partial_m\partial_n\partial_l\frac{1}{R}+\ldots. \tag{27}$$

We recognize that

$$\partial_m\partial_n\partial_l\frac{1}{R}=\left[\partial_m\partial_n\partial_l-\frac{1}{5}(\delta_{mn}\partial_l+\delta_{ml}\partial_n+\delta_{nl}\partial_m)\partial^2\right]\frac{1}{R}+\frac{1}{5}(\delta_{mn}\partial_l+\delta_{ml}\partial_n+\delta_{nl}\partial_m)\partial^2\frac{1}{R}. \tag{28}$$

The expression in the square brackets is an irreducible third-rank tensor (octupole). We shall disregard it, since the corresponding interaction leads to a mixing of atomic states having only high angular momenta, so that its contribution to the EDM of the atom or molecule is noticeably suppressed. The remaining dipole contribution to $\delta\varphi$ is of the form

$$\begin{aligned}&\delta\varphi=-Q_m\partial_m\Delta\frac{1}{R}=4\pi Q_m\partial_m\delta(\mathbf{R}),\\&H_{TP}=-e\delta\varphi=-4\pi eQ_m\partial_m\delta(\mathbf{R}),\\&Q_m=\frac{eq}{10}\left[\int\delta\rho_V r^2 r_m\,d^3r-\frac{5}{3}\langle r_m\rangle r_q^2\right]=Q\frac{I_m}{I},\\&r_q^2=\frac{1}{Z}\int\rho_0 r^2\,d^3r.\end{aligned} \tag{29}$$

Here $H_{TP}$ is the Hamiltonian of the $T$- and $P$-odd interaction of the electron with the nucleus, and $r_q^2$ is the mean squared charge radius of the nucleus. We shall hereafter call $Q$ the Schiff moment of the nucleus.

A $T$- or $P$-parity nonconserving interaction of an electron with a nucleus can be caused also by the magnetic quadrupole moment (MQM) of the nucleus.[11] In a gauge with div $\mathbf{A}=0$ the expansion of the vector potential produced by a stationary distribution of the currents in powers of $1/R$ is of the form

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

The first term of the expansion corresponds to the magnetic dipole and is of no interest to us. We transform the second term, taking into account the equality that follows from the current conservation condition $\partial_n j_n=0$:

$$0=\int\partial_p(j_p r_m r_n r_k)\,d^3r=\int[j_m r_n r_k+j_n r_m r_k+j_k r_m r_n]\,d^3r. \tag{31}$$

Since $\langle j_i r_m r_n\rangle$ contracts with a tensor that is symmetric in the indices $n$ and $m$, we have

$$^1/_2\langle j_i r_m r_n\rangle\to{}^1/_3\langle(j_i r_m-j_m r_i)r_n\rangle. \tag{32}$$

The expansion of the right-hand side of (32) in the irreducible tensors is:

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

where $a_i$ is a vector and $M_{kn}$ is a symmetric tensor. Their explicit form can be easily found from (33):

$$a_i=-\pi\int j_i r^2\,d^3r,\qquad M_{kn}=-\int(r_k\varepsilon_{npq}+r_n\varepsilon_{kpq})j_p r_q\,d^3r. \tag{34}$$

The vector potential is expressed in terms of $a$ and $M$ as follows:

$$A_i=\left[\frac{1}{4\pi}(\delta_{ik}a_l-\delta_{lk}a_i)-\frac{1}{6}\varepsilon_{ilm}M_{mk}\right]\partial_l\partial_k\frac{1}{R}. \tag{35}$$

The quantity $a$ is the anapole moment of the system, and $M$ is the magnetic quadrupole moment. For a quantum system in a state with a definite angular momentum $I$ we have

$$\begin{aligned}&\mathbf{a}=a\frac{\mathbf{I}}{I},\\&M_{mk}=\frac{3}{2}\frac{M}{I(2I-1)}\left[I_m I_k+I_k I_m-\frac{2}{3}I(I+1)\delta_{mk}\right].\end{aligned} \tag{36}$$

Comparing (34) with (36) we see that the anapole moment is the result of spatial-parity violation in $T$-parity conservation, and the MQM occurs when $P$- and $T$-invariance are simultaneously violated. The anapole moment of a nucleus was considered earlier in Ref. 29. In the present paper we consider only $P$- and $T$-odd effects.

The electromagnetic current of the nucleon takes in the nonrelativistic limit the form

$$\mathbf{j}=\frac{ie}{2m}q(\psi\nabla\psi^*-\psi^*\nabla\psi)+\frac{e\mu}{2m}[\nabla\times\psi^*\boldsymbol{\sigma}\psi], \tag{37}$$

where $m$ and $\mu$ are the mass and the magnetic moment, in nuclear magnetons, of the nucleon. We have neglected in (37) the weak dependence of the nuclear forces on the velocity. Substituting (37) in (34) we get

$$M_{kn}=\frac{e}{2m}\left\langle 3\mu\left(r_k\sigma_n+\sigma_k r_n-\frac{2}{3}\delta_{kn}\boldsymbol{\sigma}\mathbf{r}\right)+2q(r_k l_n+r_n l_k)\right\rangle. \tag{38}$$

#### a) Spherical nuclei

We consider spherical nuclei with one unpaired nucleon. With allowance for $T$- and $P$-odd interaction, the wave function of the outer nucleon is

$$\tilde{\psi}_{IM}=R_0(r)\,\Omega_{Ilm}+\beta R_1(r)\,\tilde{\Omega}_{Ilm}, \tag{39}$$

where $\Omega$ is a spherical spinor,[30] $\tilde{\Omega}=-\boldsymbol{\sigma}\cdot(\mathbf{r}/r)\Omega$ and $\beta$ is a real mixing coefficient. With the aid of (25), (29), (38), and (39) we get

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

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

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

Here

$$\langle r^n\rangle\equiv 2\beta\int R_0R_1r^{n+2}\,dr. \tag{41}$$

We note that according to (40) the MQM is due only to the anomalous magnetic moment of the nucleon. This circumstance can be quite simply verified with the aid of the Dirac equation in a spherical potential. In a nonspherical nucleus, however, the normal magnetic moment also contributes to the MQM.

It is curious that for the same reason the atom's MQM induced by the dipole moment contains, in the centrosymmetric-field approximation, an additional small quantity, the electron's anomalous magnetic moment $\alpha/2\lambda$. The MQM induced in a molecule by the EDM of an electron does not contain this smallness.

Using the Hamiltonian (19) we can calculate the mixing coefficient and the values of $\langle r^3\rangle$ and $\langle r\rangle$, say, in a Saxon-Woods potential. At first, however, we shall perform the calculations in a simple model that permits an analytic solution; this calculation turns out to be in fact no less accurate than a numerical one. Consider the motion of an unpaired nucleon in a nuclear potential $U$, neglecting the spin-orbit interaction. It is known that nuclear density and the potential $U$ are quite close in form. Assume that they coincide: $\rho(r)=U(r)\rho(0)/U(0)$. We can then rewrite (19) in the form

$$H_{TP}=\xi\sigma\nabla U,\quad \xi=\eta\frac{G}{2\sqrt{2}\,m}\frac{\rho(0)}{U(0)}\approx -2\cdot 10^{-21}\eta\ \text{[cm]}. \tag{42}$$

The total potential in which the nucleon moves is, correspondingly,

$$\tilde{U}=U+H_{TP}=U+\xi\sigma\nabla U\approx U(\mathbf{r}+\xi\sigma). \tag{43}$$

It is clear hence that the wave function, with $H_{TP}$ taken into account, is of the form

$$\tilde{\psi}=\psi(\mathbf{r}+\xi\sigma)=(1+\xi\sigma\nabla)\psi(\mathbf{r}), \tag{44}$$

where $\psi(\mathbf{r})$ is the unperturbed wave function. With the aid of (44) as well as (25), (29) and (38) we obtain

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

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

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

where

$$t_I=1\ \text{ at }\ I=l+{}^1/_2,\quad t_I=-\frac{I}{I+1}\ \text{ at }\ I=l-{}^1/_2, \tag{48}$$

$\overline{r^2}=\int|\psi|^2r^2d^3r$ is the mean squared radius of the unpaired nucleon, and $l$ is the orbital momentum of the nucleus. A numerical calculation in a Saxon-Woods potential and the experimental data on the electric and magnetic radii of the nuclei show that $\overline{r^2}$ and $r_q^2$ are nearly equal and we can put $\overline{r^2}=r_q^2=3/5R^2$, where $R=r_0A^{1/3}$ is the radius of the nucleus and $r_0=1.1$ fm. Then

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

Note that $d$ and $M$ are independent of $A$ whereas $Q$ increases like $A^{2/3}$.

It is useful to compare parametrically the EDM $d$ and $dn$ of the nucleus and of the neutron, respectively. Generally speaking, such a comparison is possible only within the framework of a definite $CP$-nonconservation scheme. There exists, however, a regular enough factor that enhances $d$ compared with $d_r$:

$$3\pi(m_\pi^2Ur_0^3)^{-1}\approx 60. \tag{50}$$

Here $(m_\pi^2\,U\,r_0^3)^{-1}$ is quite clearly of nuclear origin. The geometric factor $3\pi$ occurs when $d$ appears in the tree approximation while $d_n$ appears only in the one-loop approximation. The enhancement factor supplementing (50) in the Kobayashi-Maskawa model has a rather random numerical character. In a scheme where $CP$-nonconservation is due to a $\theta$ term (the corresponding contribution to $P$- and $T$-odd nuclear multipoles is considered in Ref. 13), the additional numerical factor leads to a noticeable decrease rather than enhancement of (50).

It is easy to verify that for an $s_{1/2}$ nucleon ($l=0, I=1/2$) Eq. (49) yields $Q=0$. The point is that we have assumed $\overline{r^2}=r_q^2$ whereas in this case, according to (46)

$$Q=-{}^1/_6eq\xi(\overline{r^2}-r_q^2), \tag{51}$$

i.e., strong mutual cancellation of the two terms takes place. We point out that a similar situation obtains for the contribution induced by the proton dipole moment proper.[28] Clearly, in the case of strong cancellation the considered analytically solvable model yields only an order-of-magnitude estimate of $Q$. Of practical importance is $^{203,205}$Tl ($3s_{1/2}$ proton), for which experimental data are available (see below). A numerical calculation in a Saxon-Woods potential yields with the aid of (19) and (40)

$$Q(\text{Tl})\approx -2\cdot 10^{-8}\eta e\ \text{[fm}^3\text{]}. \tag{52}$$

A similar calculation with Eq. (51) yields $-1.3\cdot 10^{-8}$. The result (52) is likewise of low accuracy, for according to Telitsyn's calculations[31] the difference $\overline{r^2}-r_q^2$ is quite sensitive to polarization effects and may even reverse sign if these effects are accurately taken into account (in a Saxon-Woods potential $(\overline{r^2}-r_q^2)/r_q^2=-0.13$, and according to Ref. 31 this quantity equals $0.07\pm 0.13$).

For other nuclei, according to numerical calculations in a Saxon-Woods potential, Eqs. (45), (46), (47), and (49) are approximately 50% accurate. Since this is close to the shell-model accuracy, further refinements of Eqs. (45)–(49) are meaningful only if multiparticle effects in the nucleus are

simultaneously taken into account. Numerical calculations show that corrections on the order of 50% can appear when account is taken of the nonlocal character of the nucleon-nucleon $T$- and $P$-odd interaction ($\Delta r \sim 1/m_\pi$).

According to (46) and (49), in the shell model the Schiff moment is $Q = 3$ for nuclei with an external neutron ($q = 0$). Polarization of the core leads to $q \sim 0.1$ for a neutron, so that in this case $Q$ differs from zero.

The numerical values of $d$, $Q$, and $M$ for some nuclei are listed in Table I.

### b) Nonspherical nuclei

Nonspherical nuclei are known to have close levels of opposite parity. This enhances the effects connected with the usual weak interaction. The possibility of enhancing the EDM of nonspherical nuclei when the ground state is close to a level having opposite polarity but the same angular momentum was first noted in Ref. 12 and was discussed quite recently in Refs. 8 and 13. Unfortunately, if only heavy stable nuclei are considered, the choice is quite small. We have in fact $^{161}$Dy, which has a $|5/2^-\rangle$ level at a distance 25.7 keV from the ground state $|5/2^+\rangle$, as well as $^{237}$Np (ground state $|5/2^+\rangle$, excited $|5/2^-\rangle$, $\Delta E = 59.5$ keV). There are also several nuclei with $\Delta E \sim 100$ keV ($^{153}$Eu, $^{155}$Gd, $^{163}$Dy, $^{233}$U). At first glance one might expect a noticeable enhancement of the effects compared with spherical nuclei, for which $\Delta E \sim 8$ MeV. It turns out, however, that the enhancement hardly exceeds 10 in these nuclei.

The calculation for deformed nuclei is carried out in a "frozen" (rotating with the nucleus) reference frame. The conversion to the laboratory frame is via the formulas

$$d_{\text{lab}} = \frac{J}{J+1} d_z, \quad Q_{\text{lab}} = \frac{J}{J+1} Q_z, \quad M_{\text{lab}} = \frac{J}{J+1} \frac{2J-1}{2J+3} M_{zz}. \tag{53}$$

We have taken it into account that in the ground state of the rotational band we have $J = \Omega$, where $\Omega$ is the projection of the angular momentum on the axis of the nucleus. The quantities $d_z$, $Q_z$, and $M_{zz}$ are the components of the corresponding tensors in the frozen system, the $z$ axis is directed along the nuclear axis. The contribution due to the close level is equal to

$$T = 2\langle\Omega|H_{TP}|\bar{\Omega}\rangle\langle\bar{\Omega}|\hat{T}|\Omega\rangle (E_\Omega - E_{\bar{\Omega}})^{-1}, \tag{54}$$

where $T = d_z, Q_z, M_{zz}$ is the operator of interest to us, $|\Omega\rangle$ is the ground state, and $|\bar{\Omega}\rangle$ is the state of opposite parity. We calculated the matrix elements in (54) in the Nilson single-particle oscillator model. Unfortunately, the matrix elements $d_z$, $Q_z$, and $H_{TP}$ between the nearest neighbors are small and cannot be reliably calculated. For example, the calculated matrix element $\langle 5/2^+|d_z|5/2^-\rangle$ turns out to be one-fifth the experimental value determined from the lifetime of the $|5/2-\rangle$ level of $^{161}$Dy. The matrix element $\langle\Omega|H_{TP}|\bar{\Omega}\rangle$ furthermore depends strongly on the choice of the parameters of the distribution of the density $\rho$ in the Hamiltonian (19). It appears that only the matrix element $\langle\bar{\Omega}|M_{zz}|\Omega\rangle$, which is not small, can be reliably calculated. There are good reasons for the suppression of the matrix elements $d_z$, $Q_z$, and $H_{TP}$. First, the angular momenta $I$ of the dominant components in the Nilson functions of the anomalously close states $|\Omega\rangle$ and $|\bar{\Omega}\rangle$ differ by two, and are therefore not mixed by the above operators. Second, there is a special reason, connected with its spatial structure, why the operator $H_{TP}$ is suppressed. The density and potential have like profiles also in nonspherical nuclei. Therefore if the spin-orbit interaction is neglected the approximate formula (43) is valid:

$$H_{TP} \approx \xi\sigma\nabla U = i\xi[\sigma\mathbf{P}, H_0]_-,$$

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

$$\langle\Omega|H_{TP}|\bar{\Omega}\rangle \approx i\xi\langle\Omega|[\sigma\mathbf{p}, H_0]|\bar{\Omega}\rangle \propto E_{\bar{\Omega}} - E_\Omega. \tag{55}$$

Similar factors explain the anomalous suppression of $\langle\Omega|d_z|\bar{\Omega}\rangle$ in calculations by the Nilson oscillator model. Indeed, if

$$U = \frac{m\omega_\perp^2(x^2+y^2)}{2} + \frac{m\omega_z^2 z^2}{2},$$

we have

$$d_z = er_z = \frac{e}{m\omega_z^2}\frac{\partial U}{\partial z} = \frac{ie}{m\omega_z^2}[p_z, H_0]_-. \tag{56}$$

Consequently $\langle\Omega|d_z|\bar{\Omega}\rangle$ is also proportional to the small

TABLE I. Electrodipole, Schiff, and magnetic-quadrupole moments of nuclei. The parameter $\eta$ is the coefficient in the $T$- and $P$-odd interaction Hamiltonian (19). The value given in the table for the neutron was obtained from (6b) by dividing by $\eta_n$ (20a).

| | Nucleus | Neutron | $\frac{d}{\eta}$ [e·cm]·10$^{21}$ | $\frac{Q}{\eta}$ [e·fm$^3$]·10$^8$ | $\frac{M}{\eta}\left[\frac{e}{m_p}\cdot\text{fm}\right]\cdot 10^7$ |
|---|---|---|---|---|---|
| Outer nucleon | $^{127}I_{53}$ | $p, d_{5/2}$ | 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 |
| spherical nuclei | $^{161}Dy_{66}$ | $n, 5/2^+$ | 7 | ~1 | 27 |
| | $^{237}Np_{93}$ | $p, 5/2^+$ | 1 | 4 | 20 |
| deformed | $^2H_1$ | – | 2 | 0 | 1 |
| | $^3He_2$ | – | −1 | ~0,1 | – |
| | light | – | $5\cdot 10^{-3}$ | – | – |

energy difference $E_{\bar{\Omega}} - E_{\Omega}$.

Thus, if Eqs. (55) and (56) are used literally, the contribution of the anomalously close level to $M_{zz}$ and $Q_z$ turns out to be not enhanced, and the contribution to $d_z$ is even suppressed. Actually, of course, this is not the case, since the spin-orbit interaction cannot be neglected and the potential and density profiles are not exactly similar. Numerical calculations in the Nilson model lead to the following conclusions. There is no enhancement of $d$ and $Q$ compared with spherical nuclei if the calculated values of $\langle \Omega | d_z | \bar{\Omega} \rangle$ are used. With the experimental values, however, the EDM of $^{161}$Dy is enhanced by 5–10 times (in $^{237}$Np the experimental value of $\langle \Omega | d_z | \bar{\Omega} \rangle$ is half the calculated one). The magnetic quadrupole moment in $^{161}$Dy and $^{237}$Np is enhanced by approximately one order. The calculation results are given in Table I. We emphasize once more that our calculations give only the order of magnitude of $d$, $Q$, and $M$ for deformed nuclei. These values can probably be improved by using a deformed Saxon-Woods potential.

#### c) Light nuclei. $^2$H and $^3$He

The deuteron binding energy is relatively small: $E \approx -2$ MeV. Therefore the range of the wave function exceeds greatly the radii of the strong and weak ($T$- and $P$-odd) interactions. Outside the effective range of the nuclear forces, the unperturbed wave function is

$$\psi = \chi_S \left(\frac{\varkappa}{4\pi}\right)^{1/2} \frac{e^{-\varkappa r}}{r}, \tag{57}$$

where $\varkappa = (m|E|)^{1/2}$ and $\chi_S$ is the spin wave function ($S = 1$). When account is taken of the $T$- and $P$-odd interaction (18)–(20), the wave function in the outer region takes the form

$$\tilde{\psi} = \left[1 - \gamma \frac{G}{16\sqrt{2}\, a}(\eta_1 \sigma_p - \eta_2 \sigma_n)\nabla\right]\psi, \tag{58}$$

where $a$ is the range of the forces, $\sigma_p$ and $\sigma_n$ are the proton and neutron Pauli matrices, and $\gamma$ is a dimensionless numerical factor. In the Kobayashi-Maskawa model $\eta_1 = 1.34\,\eta_0$ and $\eta_2 = -\eta_0$. Equation (58) can be derived under various model assumption, e.g., for a rectangular potential well. The parameter $\gamma$ depends on the model, but $\gamma \sim 1$ in all the cases considered by us. We point out that no suppression due to the low deuteron binding energy enters in the wave-function increment. With the aid of (58) we obtain

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

where $\mu_p$ and $\mu_n$ are the magnetic moments of the proton and neutron in nuclear magnetons. The numerical values of $d$, $Q$, and $M$ at $a = 1$ fm are listed in Table I. It can be seen that the values of $d$ and $M$ turn out to be practically the same as in heavy spherical nuclei. The same table lists estimates obtained for $^3$He with the aid of Eqs. (46) and (47).

## 4. ELECTRIC DIPOLE MOMENTS OF ATOMS AND MOLECULES

#### a) Single-particle matrix elements between electron states

The Hamiltonian of the interaction between an electron and the quadrupole field (36) is

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

Here $I$ is the angular momentum of the nucleus and $\alpha$ is the Dirac matrix for the electron. The matrix element of between single-electron states is

$$\langle \psi_2 | H_M | \psi_1 \rangle$$
$$= -\frac{3}{8}\frac{eMS}{I(2I-1)} t_{mk} \langle \Omega_2 | \sigma_m n_k + \sigma_k n_m - 2(\boldsymbol{\sigma}\mathbf{n}) n_k n_m | \Omega_1 \rangle, \tag{61}$$

where $\Omega$ is a spherical spinor corresponding to the total angular momentum $j$ of the electron, and $\mathbf{n} = \mathbf{r}/r$. The radial integral $S$ can be calculated with the aid of the quasiclassical wave functions given, e.g., in Ref. 27:

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

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

$$R_M = \frac{(j_2 - j_1 + 2)!\,(j_1 + j_2 + 3)!\,(j_1 - j_2 + 2)!\,\Gamma(\gamma_1 + \gamma_2 - 2)}{(j_1 + j_2 - 2)!\,\Gamma(\gamma_2 - \gamma_1 + 3)\,\Gamma(\gamma_1 + \gamma_2 + 3)\,\Gamma(\gamma_1 - \gamma_2 + 3)},$$
$$\varkappa = (j + 1/2)(-1)^{j + 1/2 - l}, \quad \gamma = [(j + 1/2)^2 - (Z\alpha)^2]^{1/2}, \tag{64}$$

$a_B$ is the Bohr radius, $f$ and $g$ are the upper and lower radial components of the electron bispinor, $Z_i$ is the atomic-core charge, and $\nu$ is the effective principal quantum number for the outer electron ($E = -Z_i^2 \mathrm{Ry}/\nu^2$, $\mathrm{Ry} = e^2/2a_B$). The relativistic factor $R_M$ is formulated such that $R_M \to 1$ as $Z\alpha \to 0$. In the most important case of the matrix moment $s - p_{3/2}$, the numerical factor is $x = -2/3$, $R_M(Z = 55) = 1.3$, $R_M(Z = 80) = 1.8$.

The matrix element of the electron interaction with the scalar $T$- and $P$-odd nuclear potential (2) or (29) is calculated similarly. Only the mixing of the $s$ and $p$ waves need be taken into account here, since a suppression $\sim RZ/a_B$, where $R$ is the radius of the nucleus, sets in at higher orbital momenta of the electron. If Eq. (29) is used, the matrix element for a relativistic electron diverges. With the aid of (22) we get

$$\langle s | H_{TP} | p \rangle = \frac{4Z_i^2 Z^2 e R_Q}{a_B^4 (\nu_s \nu_p)^{3/2}} Q \langle \Omega_s | \mathbf{n} | \Omega_p \rangle. \tag{65}$$

The relativistic factor $R_Q$ is different for $p_{1/2}$ and $p_{3/2}$ electrons:

$$R_{1/2} \approx \frac{4\gamma_{1/2} x_0^{2\gamma_{1/2} - 2}}{[\Gamma(2\gamma_{1/2} + 1)]^2}, \quad R_{3/2} \approx \frac{48 x_0^{\gamma_{1/2} + \gamma_{3/2} - 3}}{\Gamma(2\gamma_{1/2} + 1)\,\Gamma(2\gamma_{3/2} + 1)}, \tag{66}$$

where $x_0 = 2ZR/a_B$. With the aid of (46), (47), (64), and (65) we can compare the contributions of $Q$ and $M$ to the $T$- and $P$-odd moments of the atom:

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

where $m_e$ and $m$ are the masses of the electron and proton. It can be seen that the MQM contribution usually predominates at $I > 1/2$. Only for atoms with heavy spherical nuclei ($A > 200$) do the contributions of the Schiff moment and the MQM become comparable, all the more since $R_Q$ increases with $Z$ more rapidly than $R_M$ (at $Z = 81$ we have $R_{1/2} = 7$, $R_{3/2} = 5$ and $R_M = 1.8$). As for nonspherical nuclei, the MQM contribution for them can be enhanced by one order, as shown in the preceding section.

#### b) Induced dipole moment of atoms

We remark right away that the MQM of a nucleus contributes to the EDM only in systems with unpaired electron angular momenta. The point is that even when an electric field (the "measure" of the EDM) is turned on the magnetic field $\mathscr{H}$ of the electrons in an atom with zero angular momentum remains equal to zero (it follows from $T$-invariance that $\mathscr{H}$ cannot be proportional to $\mathscr{E}$). As a result, the MQM of the nucleus does not influence the state of the system in the linear approximation. At the same time, the mixing (65) connected with the scalar potential of the nucleus works also in systems with closed electron shells. The last circumstance is particularly important for molecules, where the electrons are usually paired.

We consider first the EDM of the cesium atom. All the necessary calculations were made in fact in Ref. 11 (see also Ref. 27), where an atom EDM induced by a proton EDM was calculated:

$$d_{Cs}^{(M)} = -\frac{4}{15} \frac{M m_e Z^2 \alpha^2 R_M r_{6s6p}}{(\nu_{6s}\nu_{6p})^{1/2}} \frac{\mathrm{Ry}}{E_{6p}-E_{6s}} \begin{cases} 1, \\ -45/28 \end{cases}$$
$$d_{Cs}^{(Q)} = \frac{16}{9} \frac{Q Z^2 (R_{1/2}+2R_{3/2}) r_{6s6p}}{a_B^2 (\nu_{6s}\nu_{6p})^{1/2}} \frac{\mathrm{Ry}}{E_{6p}-E_{6s}} \begin{cases} 1, \\ 27/28 \end{cases}. \qquad (68)$$

Here $r_{6s6p}$ is the radial integral for the amplitude $E1$ in Bohr-radius units. The upper number in the curly brackets refers to the total angular momentum of the atom $F = I + j = 4$ (and is independent of $I$), and the lower to $F = 3$. Calculation using (68), $M$ and $Q$ from Table I, and the parameters of the cesium atom (e.g., from Ref. 27) yields (in units of $e_\eta \cdot 10^{-24}$ cm) $d^{(M)} = 2.8$, $d^{(Q)} = -0.23$ at $F = 4$ and $d^{(M)} = -4.5$, $d^{(Q)} = -0.22$ at $F = 3$. It can be sseen that, just as in the effect induced by the intrinsic EDM of the proton,[11] the $d^{(M)}$ contribution predominates. From the experimental value $|d_{Cs}|/e < 3.7 \cdot 10^{-22}$ cm obtained[10] for the state $F = 4$ we get the limit $|\eta| < 130$.

The calculation is similar for the EDM of the $^{131}$Xe atom in the metastable state $5p^5 6s^3P_2$ ($E = 67068$ cm$^{-1}$), where the main contribution is also made by the MQM of the nucleus. The situation is different in the ground state of Xe, where the MQM does not work. The atom's EDM is produced here mainly by the interaction between the Schiff moment of the nucleus and the outer $5p^6$ shell. The Schiff moment determines also the EDM of the thalium atoms, since the MQM in the stable isotopes $^{203}$Tl and $^{205}$Tl is zero. Contributing to the EDM are here both the closed $6s^2$ shell and the outer $6p$ electron.

Particular interest attaches to rare-earth atoms, since their spectra contain very close levels of opposite parity. In samarium, for example, there is a metastable level $4f^6(^7F)5d\,(^8F)6s^9F_3$ ($E = 14920.45$ cm$^{-1}$) at a distance $\Delta E = 4.62$ cm$^{-1}$ from the level $4f^6(^7F)6s6p(^3P)^9G_3$ (Ref. 32). This circumstance enhances significantly the EDM in the metastable state. It can be easily estimated on the basis of the calculation for cesium. The effect in Sm is due mainly to $5d$–$6p$ mixing when an electron interacts with the MQM of the nucleus. It follows from (62)–(64) that the numerical coefficient in the single-particle matrix element (61) is in this case smaller by a factor 5–10 than for $s$–$p$ transitions. In addition, what are rally mixed are not single-particle states, but complex multiparticle states with $\sim 10$ simple components, and this weakens the effect by approximately one more order. Thus, the EDM of the metastable state of samarium exceeds that of cesium by two orders (and not by four as might be expected from a comparison of the energy intervals and the charges of the nuclei). A more accurate calculation using the wave functions of the mixing states from Ref. 32 confirms this estimate.

A nearby opposite-parity level $2p_{3/2}$ increases also the EDM in the metastable $2s$ state of deuterium: $d_D/e\eta \sim 0.5 \cdot 10^{-22}$ cm. The main contribution is made here by the magnetic quadrupole and directly by the deuteron EDM. The latter contributes because the hyperfine interaction does not satisfy the Schiff theorem. Experiments with deuterium are inconvenient because an electric field causes emission of the $2s$ level.

The calculated EDM of the atoms are listed in Table II.

#### c) Induced dipole moment of molecules

It was shown in Refs. 28, 33, and 34 that $T$- and $P$-nonconservation in polar molecules is greatly enhanced because of the small interval between rotational levels of opposite parity. We consider first diatomic molecules with paired electron momenta. As already noted, the MQM of the nucleus does not work in them and the EDM of a molecule in a

TABLE II. EDM of atoms

| Atom | $^{133}$Cs | | $^{131}$Xe | | $^{203,205}$Tl | $^{147,149}$Sm |
|---|---|---|---|---|---|---|
| State | $F=3$ | $F=4$ | ground | $^3P_2$, $F=7/2$ | $F=1$ | $E=14920$ cm$^{-1}$ |
| $\frac{d}{\eta}\cdot 10^{24}$, $e\cdot$cm | −4,7 | 2,6 | ~0,01 | −0,7 | 0,3 | ~200 |

stationary state is the result of the Schiff moment. To explain how the constraint on the $T$- and $P$-odd interaction constant can be deduced from experiments on observing $T$-invariance in the TlF molecule[5-7] we consider a simple model of the electronic structure of this molecule. We shall assume that an outer electron goes over from the Tl atom to the F atom. The distance between nuclei is $r_e = 3.91a_B$.[35] As a result, the $Tl^+$ ion is in an electric field $\mathscr{E} = e/r_e^2$, which polarizes the outer $6s^2$ shell. Therefore the single-particle orbitals become mixtures of $6s$ and $6p$ states:

$$|\omega\rangle = |6s, \omega\rangle + \beta\left[-\frac{2\omega}{\sqrt{3}}|6p_{1/2}, \omega\rangle + \sqrt{\frac{2}{3}}|6p_{3/2}, \omega\rangle\right], \qquad \beta = \frac{2}{\sqrt{3}}\frac{\mathrm{Ry}}{E_{6s}-E_{6p}}\frac{r_{6s6p}}{r_e^2} = 0.27. \tag{69}$$

Here $r_{6s6p}$, $E_{6s}$ and $E_{6p}$ are the radial integral and the energies in $Tl^+$. The quantities $r_{6s6p}$ and $r_e$ are in units of $a_B$, and $\omega = \pm 1/2$ is the projection of the single-electron angular momentum on the molecule axis. With the aid of (69) and (65) we find the effective Hamiltonian of the $T$- and $P$-odd interaction of the Tl spin with the molecule axis N:

$$\frac{H_{eff}}{\mathrm{Ry}} = \frac{32}{3\sqrt{3}}\beta\frac{Z_i^2Z^2(R_{1/2}+2R_{3/2})}{(\nu_{6s}\nu_{6p})^{3/2}}\frac{\mathbf{Q}}{ea_B^3}\mathbf{N} = 1.1\cdot 10^5\frac{\mathbf{Q}}{ea_B^3}\mathbf{N}. \tag{70}$$

The effective $Tl^+$ charge is $Z_i = 2$, $\nu_{6s} = 1.63$, $\nu_{6p} = 2.15$ ($E = -Z_i^2\,\mathrm{Ry}/\nu^2$), and $r_{6p6s} = 2.3$. A more accurate calculation[8] yields a result 2.5 times smaller than (70). Taking this into account and using the value of $Q_{Tl}$ from Table I, we get

$$H_{eff}(\mathrm{TlF}) = \mathrm{Ry}\,\varkappa_{Tl}(\mathbf{I}/I)_{Tl}\mathbf{N}, \quad \varkappa_{Tl} = -0.6\cdot 10^{-17}\eta. \tag{71}$$

The subscript Tl signifies that we are dealing with the interaction of the Tl spin with the molecule axis. The best of the experimental limits of the constant $\varkappa_{Tl}$ is[7]

$$\varkappa_{Tl}\,\mathrm{Ry} = 2\pi\hbar(8\pm 12)\cdot 10^{-3}\,\mathrm{Hz}. \tag{72}$$

From (71) and (72) follows

$$\eta = -0.4\pm 0.6. \tag{73}$$

The estimate (71) is valid also for Tl compounds with other halogens, since they have similar electron structures. In the TlI molecule, the interacion of the spin of the iodine nucleus with the molecule axis becomes noticeable. We shall estimate its magnitude, using the calculation[8] for th TlF molecule and taking into account the regular growth factor as $Z$ increases from fluorine to iodine: $Z^2(R_{1/2} + 2R_{3/2})$ (see (65)). This yields

$$H_{eff} = -0.16\cdot 10^5\,\mathrm{Ry}\frac{\mathbf{Q}}{ea_B^3}\mathbf{N} = \mathrm{Ry}\,\varkappa_I\left(\frac{\mathbf{I}}{I}\right)_I\mathbf{N}, \qquad \varkappa_I = 0{,}15\cdot 10^{-17}\eta. \tag{74}$$

Comparing (74) and (71) we see that the contribution of the Tl nucleus still seems to predominate here.

The kinetics of $\varkappa_{Bi}$ in the molecule TiF (Cl, Br, I) is approximately the same as that of $\varkappa_{Tl}$ in TlF (Cl, Br, I). It appears also that $\varkappa_{Np}$ in the NpF molecule is 4–6 times larger, owing to the larger $Z$ and $Q$ of the neptunium nucleus (if such a molecule exists and has a simple enough electronic structure).

Consider finally the CsI molecule, which is apparently most convenient from the experimental point of view. Here, too, in first-order approximation the iodine atom has one extra electron, and with respect to the electron wave function near I this molecule is similar to TlI. One should therefore expect $\varkappa_I$ to be approximately of the same order as in TlI. The value of $\varkappa_{Cs}$ is of the same order. The larger of the two values of the constants for the considered molecules are given in Table III. We emphasize that these values are in fact estimates accurate to within a factor 2–3.

We calculate now the $T$- and $P$-odd EDM of a molecule in a stationary rotational state. The experiment is performed in a magnetic field that breaks up the hyperfine structure due to the interaction between the nuclear magnetic moment and the rotational one. The wave function of the molecule can therefore be represented by the product

$$|\psi\rangle = |I, I_z)\,|L, L_z\rangle, \tag{75}$$

where $L$ is the rotational moment of the molecule. The EDM is produced in the state (75) on account of $T$- and $P$-odd mixing by the interaction $H_{\mathrm{eff}} = \varkappa\mathrm{Ry}\,\mathbf{N}\cdot\mathbf{I}/I$ of the opposite-parity rotational states:

$$d_z = \sum_{L',L_z'} 2\langle II_z|\langle LL_z|H_{eff}|L'L_z'\rangle|II_z'\rangle \times\langle II_z'|\langle L'L_z'|D_{\mathrm{mol}}N_z|LL_z\rangle|II_z\rangle$$

$$\times(E_L-E_{L'})^{-1} = 2\varkappa\,\mathrm{Ry}\,D_{\mathrm{mol}}\frac{I_z}{I}\sum_{L'}\frac{|\langle LL_z|N_z|L'L_z\rangle|^2}{E_L-E_{L'}} = \frac{\varkappa\,\mathrm{Ry}}{B}D_{\mathrm{mol}}\frac{I_z}{I}\frac{L(L+1)-3L_z^2}{L(L+1)(2L-1)(2L+3)}. \tag{76}$$

Here $D_{\mathrm{mol}}$ is the dipole moment of the polar molecule in its rest system (see Refs. 35 and 36), and $E_L = BL(L+1)$. Equation (76) is valid in not too strong an electric field: $D_{\mathrm{mol}}\mathscr{E} \ll 2B(L+1)$. In an arbitrary field, the Stark energy shift can be obtained from the plots of $\langle N_z\rangle$ in Ref. 37. The electric dipole moment is a maximum at $L = 0$ and $I_z' I$:

TABLE III. Constant of $T$- and $P$-odd interaction of nuclear spin with molecule axis [see (71)] and EDM of molecules in the ground state

| | TlF | TlI | BiF | BiI | NpF | NpI | CsF | CsI |
|---|---|---|---|---|---|---|---|---|
| $\lvert\varkappa/\eta\rvert\cdot 10^{17}$ | 0,6 | 0,6 | 0,6 | 0,6 | ~3 | ~3 | 0,15 | 0,15 |
| $\lvert d/\eta\rvert\cdot 10^{20}$, $e\cdot$cm | 0,9 | 7 | 0,9 | 7 | ~4 | ~30 | 0,5 | 5 |

$$d=-(\varkappa\ \mathrm{Ry}/3B)D_{\mathrm{mol}}. \qquad (77)$$

The numerical values of $d$ for the molecules considered are given in Table III. Because of the smaller rotational interval, the EDM of iodine compounds exceeds that of fluorine compounds. This advantage vanishes however in an electric field $\mathscr{E}\sim 5$–$10$ kV/cm, for beyond this the growth of the molecule polarization is practically stopped.

We consider now molecules with unpaired electron angular momenta. The dominant effect here is that of the MQM of the nucleus. We take by way of example the molecule $^{201}$HgF. The electronic state of this molecule is $^2\Sigma$. It is known that for such states the electron spin can be regarded as split off from the molecule axis, so that in the rest system only the wave function of the electron orbital motion need be considered. We obtain this wave function under the assumption that one outer electron of the mercury atom goes over to F. The wave function of the remaining electron is [cf. (69)]

$$|\Sigma\rangle=|6s\rangle+\beta|6p\rangle, \qquad \beta=\frac{2}{\sqrt{3}}\frac{\mathrm{Ry}}{E_{6s}-E_{6p}}\frac{r_{6s6p}}{r_e^2}\approx 0.27. \qquad (78)$$

Now, regarding the expression in the angle brackets in (61) as an operator, we obtain with the aid of (78) the effective Hamiltonian

$$\frac{H_{eff}}{\mathrm{Ry}}=\frac{Mm_e}{ea_B}\frac{Z_i^2Z^2\alpha^2\mathrm{R}_M}{2(\nu_{6s}\nu_{6p})^{3/2}}\frac{t_{mk}\sigma_l}{I(2I-1)}$$

$$\times\langle\Sigma|\delta_{lm}n_k+\delta_{lk}n_m-2n_ln_kn_m|\Sigma\rangle$$

$$=\frac{2\sqrt{3}\beta}{5}\frac{Mm_e}{ea_B}\frac{Z_i^2Z^2\alpha^2R_M}{(\nu_{6s}\nu_{6p})^{3/2}}\frac{t_{mk}\sigma_mN_k}{I(2I-1)}. \qquad (79)$$

Equation (79) was derived with allowance for the equality

$$\langle\Sigma|\delta_{lm}n_k+\delta_{lk}n_m-2n_ln_kn_m|\Sigma\rangle$$

$$=\frac{2\sqrt{3}}{5}\beta\left[\delta_{lm}N_k+\delta_{lk}N_m-\frac{2}{3}\delta_{mk}N_l\right].$$

The magnetic interaction of the electron spin with the nuclear spin causes the stationary state to have fixed $F$, where $\mathbf{F}=\mathbf{I}+\mathbf{s}$. Recognizing that

$$\langle F|t_{mk}\sigma_m|F\rangle=AF_k, \qquad (80)$$

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

$$x=F(F+1)-I(I+1)-\frac{3}{4},$$

we transform from (79) to the effective Hamiltonian

$$H_{eff}=\mathrm{Ry}\,\varkappa(\mathbf{F}/F)\mathbf{N}, \qquad (81)$$

$$\varkappa=\frac{4\beta}{5\sqrt{3}}\frac{Mm_e}{ea_B}\frac{Z_i^2Z^2\alpha^2R_M}{(\nu_{6s}{}^3\nu_{6p}{}^3)^{1/2}}\begin{cases}1, & F=I+1/2\\ -\dfrac{(I+1)(I+3/2)}{I(I+1/2)}, & F=I-1/2\end{cases}$$

For $Hg^+$ we have $R_M=1.8$, and the parameters $Z_i$, $\nu_{6s}$, $\nu_{6p}$ and $r_{6p6s}$ are practically the same as for $Tl^+$ (see the calculation for TlF). We assume that, just as for TlF, Eq. (81) overestimates the answer by 2.5 times. As a result we have

$$\varkappa_{\mathrm{Hg}}=-3\cdot10^{-17}\eta\begin{cases}-0{,}4, & F=2\\ 1, & F=1\end{cases}. \qquad (82)$$

The results of an analogous calculation for the molecules BaF and BaI are given in Table IV. Owing to the large MQM of the $^{161}$Dy and $^{237}$Np nuclei (see Table I) we can expect for DyF and NpO a value of $\varkappa$ about 20 times larger than for HgF, provided, of course, that these molecules have a sufficiently simple electronic structure. We calculate now the $T$- and $P$-odd dipole moments of molecules with unpaired electron spin in a definite rotational state. We assume that in first-order approximation the rotation is split off from $F$, and $F,|\psi\rangle=|F,F_z\rangle|L,L_z\rangle$. We then get in analogy with (76)

$$d_z=\frac{\varkappa\,\mathrm{Ry}}{B}D_{\mathrm{mol}}\frac{F_z}{F}\frac{L(L+1)-3L_z^2}{L(L+1)(2L-1)(2L+3)}; \qquad (83)$$

at $L=0$ and $F_z=F$ we have

$$d=-(\varkappa\ \mathrm{Ry}/3B)D_{\mathrm{mol}}.$$

The numerical values of $d$ are given in Table IV. For the molecules BiO and BiS, owing to the strong coupling of the electron spin with the molecule axis, the calculation described cannot be used literally. One can nevertheless expect for these molecules, in lower rotational states, the EDM to be the same or even somewhat larger than for HgF ($d/\eta e\sim 10^{-19}$ cm).

## 5. CONCLUSION

Regular enhancement of the $T$- and $P$-odd multipoles in atomic nuclei adds greatly to the real physical significance of experimental searches for $T$-nonconservation in atoms and molecules. Whereas the disparity of the experimental constraints (1) and (2) on the nucleon EDM reaches three orders of magnitude, the constraints on the superweak interaction constant $\eta$ differ by only one order [compare (1) with (6b) and (73) with (20a)]. Moreover, by merely going from TlF to other compounds, without increasing the absolute experimental accuracy, an advance by 1–2 orders would be possible. The dipole moments of the compounds of dysprosium and nep-

TABLE IV. Constant of $T$- and $P$-odd interaction of the angular momentum $F=I+s$ with the axis [see (81)] and EDM of radicals at $F=I-s$.

| | BaF | BaI | HgF | HgI | DyF | DyI | NpO | NpS |
|---|---|---|---|---|---|---|---|---|
| $\lvert\varkappa/\eta\rvert\cdot10^{17}$ | 0,6 | 0,6 | 3 | 3 | ~50 | ~50 | ~50 | ~50 |
| $\lvert d/\eta\rvert\cdot10^{20}$, $e$·cm | 1,5 | 15 | 4 | 30 | ~70 | ~500 | ~70 | ~150 |

tunium, expected in the Kobayashi-Maskawa model (see Table IV), are close to the sensitivity of the experiements aimed at finding the neutron EDM. Although diatomic molecules of dysprosium and neptunium are difficult to synthesize, one can imagine that these molecules can enter in more complicated compounds, some of which may be volatile (see Ref. 38). We recall that dysprosium has a stable isotope, and neptunium an almost stable one, and in both the $T$-odd moments are additionally enhanced by approximately an order because the nucleus contains close levels of opposite parity.

As for atomic experiments, the efficiency might be increased here by approximately two orders by going to metastable states of rare-earths, where anomalously low energy intervals between levels of opposite parity are encountered. On the other hand, the obvious experimental advantages offered by the ordinary atomic xenon in the ground state could offset with large margin the suppression of the effect in it compared, say, with atomic cesium.

Moreover, the experiment might be performed with liquid xenon. We wish in this connection to call attention again to the possibility of searching for $T$-nonconservation with the aid of NMR in the liquid phase. This possibility was discussed earlier in Ref. 39.

Of particular interest might be experiments such as on NMR in ferroelectrics, where the effective electric field acting on the nuclear one is not much weaker than the atomic field. In other words, we have here an effect enhancement of the same type as in diatomic polar mlecules.

Finally, in experiments with superfluid $^3$He in the polarized $A_1$ phase one might hope to measure the EDM of the $^3$He nucleus at a level $\sim e \cdot 10^{-27}$ cm (Ref. 40). As seen from Table I, this figure is only two orders of magnitude larger than the prediction of the Kobayashi-Maskawa model.

Thus, atomic and molecular experiments undoubtedly possess some still unexplored possibilities for serious progress in the investigations of the nature of $CP$-nonconservation.

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