Collective *T*- and *P*-Odd Electromagnetic Moments in Nuclei with Octupole Deformations

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Parity and time invariance violating forces produce collective *P*- and *T*-odd moments in nuclei with static octupole deformation. Collective Schiff moment, electric octupole and dipole, and also magnetic quadrupole appear due to the mixing of rotational levels of opposite parity and can exceed single-particle moments by more than a factor of 100. This enhancement is due to two factors, the collective nature of the intrinsic moments and the small energy separation between members of parity doublets. The above moments induce *T*- and *P*-odd effects in atoms and molecules. Experiments with such systems may improve substantially the limits on time reversal violation. [S0031-9007(96)00352-3]

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Parity and time invariance nonconserving nuclear moments induced by *P*-, *T*-odd nuclear forces were discussed, e.g., in Refs. [1–6]. These moments can be enhanced in nuclei which have close to the ground state (g.s.) levels of the same spin as the g.s. but opposite parity [3,4]. An interesting possibility to enhance the effect is to consider mechanisms producing collective *T*-, *P*-odd moments. In Ref. [7] it was shown that the "spin hedgehog" mechanism produces a collective magnetic quadrupole. In the present paper we want to consider a different mechanism: mixing of opposite parity rotational levels (parity doublets) by *T*-, *P*-odd interaction in the nuclei with octupole deformation. This deformation was demonstrated to exist in nuclei from the Ra-Th and Ba-Sm region and produces such effects as parity doublets, large dipole and octupole moments in the intrinsic frame of reference, and enhanced $E1$ and $E3$ transitions (see review [8]).

Let us start our consideration from the expression for the electrostatic potential of a nucleus screened by the electrons of the atom. If we consider only the dipole *T*-, *P*-odd part of screening (Purcell-Ramsey-Schiff theorem [9]) one finds [4]

$$\varphi(\boldsymbol{R}) = \int \frac{e\rho(\boldsymbol{r})}{|\boldsymbol{R}-\boldsymbol{r}|}\, d^3\boldsymbol{r} + \frac{1}{Z}(\boldsymbol{d}\nabla)\int \frac{\rho_s(r)}{|\boldsymbol{R}-\boldsymbol{r}|}\, d^3\boldsymbol{r}\,. \tag{1}$$

Here $\rho(\boldsymbol{r})$ is the nuclear charge density $\int \rho(\boldsymbol{r}) d^3\boldsymbol{r} = Z$, $\rho_s(r)$ is spherically symmetric part of $\rho(\boldsymbol{r})$, and $\boldsymbol{d} = \int e\boldsymbol{r}\rho(\boldsymbol{r})\, d^3\boldsymbol{r}$ is the electric dipole moment (EDM) of the nucleus. The multipole expansion of $\varphi(\boldsymbol{R})$ contains both *T*-, *P*-even and *T*-, *P*-odd terms. The dipole part in Eq. (1) is canceled out by the second term in this equation,

$$-\int e\left(\boldsymbol{r}\nabla\frac{1}{R}\right)\rho(\boldsymbol{r})\, d^3\boldsymbol{r} + \frac{1}{Z}(\boldsymbol{d}\nabla)\frac{1}{R}\int \rho_s(r)\, d^3\boldsymbol{r} = 0\,. \tag{2}$$

The next term is the electric quadrupole which is *T*-, *P*-even thus the first nonzero *T*-, *P*-odd term is

$$\varphi^{(3)} = -\frac{1}{6}\int e\rho(\boldsymbol{r}) r_\alpha r_\beta r_\gamma\, d^3\boldsymbol{r}\, \nabla_\alpha\nabla_\beta\nabla_\gamma \frac{1}{R} + \frac{1}{2Z}(\boldsymbol{d}\nabla)\nabla_\alpha\nabla_\beta \frac{1}{R}\int \rho_s(r) r_\alpha r_\beta\, d^3\boldsymbol{r}\,. \tag{3}$$

Here $r_\alpha r_\beta r_\gamma$ is a reducible tensor. After separation of the trace there will be terms which will contain a vector $\boldsymbol{S}$ (Schiff) and a rank 3, $Q_{\alpha\beta\gamma}$ (electric octupole) moments [4],

$$\begin{aligned} \varphi^{(3)} &= \varphi^{(3)}_{\text{Schiff}} + \varphi^{(3)}_{\text{octupole}}\,, \\ \varphi^{(3)}_{\text{Schiff}} &= -\boldsymbol{S}\nabla\Delta\frac{1}{R} = 4\pi\boldsymbol{S}\nabla\delta(R), \\ \varphi^{(3)}_{\text{octupole}} &= -\frac{1}{6}Q_{\alpha\beta\gamma}\nabla_\alpha\nabla_\beta\nabla_\gamma\frac{1}{R}\,, \end{aligned} \tag{4}$$

where

$$\boldsymbol{S} = \frac{1}{10}\left(\int e\rho(\boldsymbol{r})r^2\boldsymbol{r}\, d^3\boldsymbol{r} - \frac{5}{3}\boldsymbol{d}\frac{1}{Z}\int \rho_s(r)r^2\, d^3\boldsymbol{r}\right) \tag{5}$$

is the Schiff moment (SM) and

$$\begin{aligned} Q_{\alpha\beta\gamma} &= \int e\rho(\boldsymbol{r}) \\ &\quad\times [r_\alpha r_\beta r_\gamma - \tfrac{1}{5}(\delta_{\alpha\beta}r_\gamma + \delta_{\beta\gamma}r_\alpha + \delta_{\alpha\gamma}r_\beta)]\, d^3\boldsymbol{r}\,, \\ Q_{zzz} &\equiv \frac{2}{5}Q_3 = \frac{2}{5}\sqrt{\frac{4\pi}{7}}\int e\rho(\boldsymbol{r})r^3 Y_{30}\, d^3\boldsymbol{r} \end{aligned} \tag{6}$$

is a tensor octupole moment.

Here we will consider the collective SM, collective octupole, and also collective dipole as well as the collective magnetic quadrupole resulting from the rotation of the dipole. The mechanism for collective SM, dipole, and octupole is the following: collective moments in the body-fixed system of the deformed nucleus are assumed to exist without any T, P violation. However, without T, P violation the average value of these moments for a rotational state in the laboratory system is zero. *T*-, *P*-odd mixing of rotational doublet states produces an average orientation of the nuclear axis $\boldsymbol{n}$ along nuclear spin $\boldsymbol{I}$. In the case of a nearly degenerate rotational doublet

$$\Psi^{\pm} = \frac{1}{\sqrt{2}}(|IMK\rangle \pm |IM - K\rangle), \tag{7}$$

where $K = \boldsymbol{I}\boldsymbol{n}$. If the T, P interaction mixes the members of the doublet with the coefficient α, the total wave function is $\Psi = \Psi^{+} + \alpha\Psi^{-}$ or

$$\Psi = \frac{1}{\sqrt{2}}[(1 + \alpha)|IMK\rangle + (1 - \alpha)|IM - K\rangle], \tag{8}$$

one obtains

$$\langle\Psi|n_z|\Psi\rangle = 2\alpha\frac{KM}{(I + 1)I}. \tag{9}$$

The intrinsic electric dipole and Schiff moments are directed along $\boldsymbol{n}$, $\boldsymbol{d} = d\boldsymbol{n}$ and $\boldsymbol{S} = S\boldsymbol{n}$, and therefore have nonzero average values in the g.s. $M = K = I$.

To elucidate the origin of collective T-, P-odd moments consider a simple classical "molecular" model, shown in Fig. 1: two charges Zq and q with masses $Z'm$ and m have coordinates $x_1 = -a$ and $x_2 = Z'a$ so the center of mass is at $x = 0$. This "molecule" has dipole, quadrupole, octupole, and Schiff moments. The electric dipole in this case is $d = (Z - Z')aq$. Consider $Z' = Z$, in this case $d = 0$, but the SM and octupole moment are not zero. The octupole moment Q_3 is proportional to $Z - 1$ (for $Z = 1$ there is only quadrupole deformation). SM in the body-fixed frame is

$$S = \frac{1}{10}qa^3Z(Z^2 - 1). \tag{10}$$

For $I = \frac{1}{2}$ the SM is not equal to zero ($S \neq 0$) as opposed to the octupole moment which vanishes because one cannot satisfy angular momentum coupling. Thus the octupole deformation is hidden. It is possible to have a situation in which $d = 0$, $Q_3 = 0$ in the laboratory system but the SM in the laboratory is $S \neq 0$. This result applies to any system, for example, to an elementary particle (neutron, electron). Indeed, for spin $s = \frac{1}{2}$ there is only one T-, P-odd form factor [10,11]. However, we have shown that the two moments, EDM and SM, are not necessarily related to each other. There is no contradiction here. The relativistic expression for the T-, P-odd electromagnetic current for $s = \frac{1}{2}$ in momentum representation is

$$j_\mu = f(q^2)\bar{\psi}\gamma_5\sigma_{\mu\nu}iq_\nu\psi, \tag{11}$$

where q is the momentum transfer, γ_5 and $\sigma_{\mu\nu}$ are Dirac matrices. The form factor can be expanded

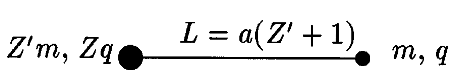

FIG. 1. A "molecular" model of octupole deformation: two charges Zq and q with masses $Z'm$ and m placed at $-a$ and $Z'a$ with respect to the center of mass.

$$f(q^2) = d + f'(0)q^2 + \cdots, \tag{12}$$

where $d = f(0)$ is the electric dipole moment of the particle [6]. In the nonrelativistic limit

$$j_0 = -f(q^2)i\psi^\dagger\boldsymbol{\sigma}\boldsymbol{q}\psi. \tag{13}$$

The electric potential produced by this current is

$$\varphi(q^2) \equiv j_0D_{0\nu} = -4\pi i\frac{\boldsymbol{\sigma}\boldsymbol{q}}{q^2}[d + f'(0)q^2 + \cdots], \tag{14}$$

where $D_{\mu\nu} = 4\pi g_{\mu\nu}/q^2$ is the photon propagator. In the coordinate representation

$$\varphi(r) = d\boldsymbol{\sigma}\nabla\frac{1}{r} + 4\pi f'(0)\boldsymbol{\sigma}\nabla\delta(\boldsymbol{r}) + \cdots. \tag{15}$$

The first term in $\varphi(r)$ gives the long-range dipole field while the second term is the contact field of the SM, i.e., $\boldsymbol{S} \sim f'(0)\boldsymbol{\sigma}$ [see Eq. (4)]. Thus, the SM emerges from the same form factor as the electric dipole. One can therefore have *a priori* a situation in which T, P is violated, the Schiff moment is not zero, but the dipole moment of the particle is zero.

The mechanism of rotational level mixing can also produce a magnetic quadrupole. Indeed, in the intrinsic frame of reference a deformed nucleus can have both a magnetic dipole and magnetic quadrupole without T, P violation. Then T-, P-odd interaction mixes rotational parity doublets and can produce magnetic quadrupole in the mixed state. It is also worth noting that higher T-, P-odd moments can appear due to rotation of lower moments. For example, rotating electric dipole produces magnetic quadrupole. However, all these contributions to higher moments will be proportional to L_z/M_Ac where M_A is a large mass of the nucleus and consequently very small.

The intrinsic moments of heavy deformed nuclei are well described using the two-fluid liquid drop model [12–14]. We consider here even-odd nuclei, so electric moments, except the dipole, are determined by the moments of the even Z core. The surface of a deformed nucleus is

$$R = R_0\left(1 + \sum_{l=1}\beta_lY_{l0}\right). \tag{16}$$

The β_1 deformation is determined from the requirement that the center of mass fixed at $z = 0$, i.e., $\int zd^3\boldsymbol{r} = 0$,

$$\beta_1 = -3\sqrt{\frac{3}{4\pi}}\sum_{l=2}\frac{(l + 1)\beta_l\beta_{l+1}}{\sqrt{(2l + 1)(2l + 3)}}. \tag{17}$$

The proton density in case of deformed nucleus is [12]

$$\rho = \frac{\rho_0}{2} - \frac{\rho_0}{8}\frac{e^2Z}{CR_0} \times\left[\frac{3}{2} - \frac{1}{2}\left(\frac{r}{R_0}\right)^2 + \sum_{l=1}\frac{3}{2l + 1}\left(\frac{r}{R_0}\right)^l\beta_lY_{l0}\right], \tag{18}$$

where $\rho_0 = 3A/4\pi R_0^3$ and C is the volume symmetry-energy coefficient. The dipole moment generated by this proton distribution is in the lowest order of deformation [12–14]

$$d_{\rm intr} = eAZ\frac{e^2}{C}\frac{3}{40\pi}\sum_{l=2}\frac{(l^2-1)(8l+9)}{[(2l+1)(2l+3)]^{3/2}}\beta_l\beta_{l+1}. \quad (19)$$

The inclusion of the neutron skin effect as well as the shell correction reduces somewhat $d_{\rm intr}$, nevertheless Eq. (19) with the $C \simeq 20-30$ MeV fits experimental values quite well [12,14]. This moment appears only because the Coulomb force produces a relative shift of protons versus neutrons. The constant part of the density in Eq. (18) does not contribute to $d_{\rm intr}$. The intrinsic Schiff moment turns out to be

$$S_{\rm intr} = eAR_0^3\frac{3}{40\pi}\left(1-\frac{e^2Z}{R_0C}\frac{19}{70}\right)\times\sum_{l=2}\frac{(l+1)\beta_l\beta_{l+1}}{\sqrt{(2l+1)(2l+3)}}. \quad (20)$$

(Note that in the liquid drop model $A/2$ times the expression in the parentheses is about Z.) Here the constant part of ρ in Eq. (18) gives the main contribution (about 90% in nuclei with $Z \sim 90$). The expression for the intrinsic octupole moment is [15]

$$Q_{3\rm intr} = eZR_0^3\frac{3}{2\sqrt{7\pi}}\left(\beta_3+\frac{2}{3}\sqrt{\frac{5}{\pi}}\beta_2\beta_3+\cdots\right). \quad (21)$$

The P- and T-odd potential has the form [4,16]

$$V^{PT} = \frac{G}{\sqrt{2}}\frac{\eta}{2m}\rho_0\sum_i\boldsymbol{\sigma}_i[\boldsymbol{\nabla}_if(\boldsymbol{r}_i)], \quad (22)$$

where $G = 10^{-5}/m^2$ is the Fermi constant and $\rho_t(\boldsymbol{r}) = \rho_0 f(\boldsymbol{r})$ is the nuclear density.

We use here the particle-core model for a reflection-asymmetric nucleus [17,18]. The T-, P-odd as well as P-odd, T-even mixing was studied in this model recently [19]. The wave functions in the model are [17,19]

$$\Psi_{MK}^{Ip} = \left[\frac{2I+1}{16\pi^2}\right]^{1/2}[1+\hat{R}_2(\pi)]D_{MK}^I\Phi_K^p, \quad (23)$$

where $\hat{R}_2(\pi)$ denotes rotation through an angle π about the intrinsic 2 axis. The $\Phi^p \equiv \Phi^{\pm}$ are particle-core intrinsic states of good parity p. Denoting the good parity core states χ^π and particle states ϕ^π we write

$$\Phi^+ = a_+\chi^+\phi^+ + b_+\chi^-\phi^-,$$
$$\Phi^- = a_-\chi^-\phi^+ + b_-\chi^+\phi^-. \quad (24)$$

The states χ^π are projections of the reflection-asymmetric states χ_A [17]

$$\chi^\pi = \frac{1}{\sqrt{2}}(1+\pi\hat{P})\chi_A. \quad (25)$$

The matrix elements of V^{PT} are [19]

$$\langle\Psi_{MK}^{I+}|V^{PT}|\Psi_{MK}^{I-}\rangle = a_+b_-\langle\phi_K^+|V^{PT}|\phi_K^-\rangle + a_-b_+\langle\phi_K^+|V^{PT}|\phi_K^-\rangle. \quad (26)$$

Note that the pseudoscalar operator V^{PT} cannot connect states of an even-even axially symmetric core χ^π [19]. The expectation value of a T-, P-odd operator $\hat{O}$ in a T-, P-admixed state $\tilde{\Phi}_i^+$ is

$$\langle\tilde{\Phi}_i^+|\hat{O}|\tilde{\Phi}_i^+\rangle = 2\alpha_{ii}\langle\Phi_i^+|\hat{O}|\Phi_i^-\rangle + 2\sum_{j\neq i}\alpha_{ij}\langle\Phi_i^+|\hat{O}|\Phi_j^-\rangle. \quad (27)$$

The matrix elements between core states are

$$\langle\chi^+|\hat{O}|\chi^-\rangle = \langle\chi_A|\hat{O}|\chi_A\rangle. \quad (28)$$

Writing the one-body operator $\hat{O}$ as the sum of core and particle parts $\hat{O} = \hat{O}_{\rm core} + \hat{O}_{\rm p}$ one obtains

$$\langle\Phi_i^+|\hat{O}|\Phi_j^-\rangle = \langle\chi_A|\hat{O}_{\rm core}|\chi_A\rangle(a_{+i}a_{-j}+b_{+i}b_{-j}) + \langle\phi_i^+|\hat{O}_p|\phi_j^-\rangle(a_{+i}b_{-j}+a_{-i}b_{+j}). \quad (29)$$

The contribution of the single neutron is small for the SM operator and is absent for the octupole moment. In the case of closely spaced doublets $a_{+i} \approx a_{-i}$, $b_{+i} \approx b_{-i}$, and $a_{+i}a_{-j} + b_{+i}b_{-j} \approx \delta_{ij}$. The expressions for the expectation values of a T-, P-odd operator of rank l in the body-fixed and laboratory systems become

$$\langle\tilde{\Phi}_i^+|\hat{O}|\tilde{\Phi}_i^+\rangle \approx 2\alpha_{ii}\langle\chi_A|\hat{O}_{\rm core}|\chi_A\rangle,$$
$$\langle\tilde{\Psi}_{MK}^{I+}|\hat{O}|\tilde{\Psi}_{MK}^{I+}\rangle = \langle III0|II\rangle^2\langle\tilde{\Phi}_i^+|\hat{O}|\tilde{\Phi}_i^+\rangle. \quad (30)$$

Currently, the best limits on Schiff moments and the coupling constants of T-, P-violating nucleon-nucleon interactions are obtained from the measurements of the electric dipole moments in ^{199}Hg, ^{129}Xe [20] atoms and TlF molecule [21,22]. Nuclei of these atoms do not have octupole deformation. However, similar experiments can be done with heavy atoms (Ra, Rn) which are electronic structure analogs of these atoms but their nuclei have octupole deformation.

Our calculations were performed for relatively long lived even-odd isotopes ^{223,225}Ra and ^{223}Rn. Variants of the model used here are shown to describe quite well the g.s. parity doublets in the Ra-Th region [8,17,23]. We used here the same version as in Ref. [19], the deformation and core parity splitting parameters were taken from Ref. [17,23]. The calculations of the mixing coefficients were performed using Nilsson potential. The ^{223,225}Ra and ^{223}Rn have the g.s. $\frac{3}{2}+$, $\frac{1}{2}+$, and $\frac{7}{2}$. The octupole deformation for all these isotopes is $\beta_3 \approx 0.1$. Our results are shown in Table I. The mixing coefficients in our calculations are in the range $(0.6-7)\times10^{-7}\eta$. The Schiff moments of the reflection-asymmetric nuclei in the intrinsic system are in the range 22–29 e fm^3. Correspondingly the T-, P-odd Schiff moments [Eq. (30)]

TABLE I. Admixture coefficients α (absolute values), experimental energy splitting between the g.s. doublet levels $\Delta E = E^- - E^+$, *intrinsic* Schiff moments, and Schiff moments as well as induced atomic dipole moments. The values for ^{199}Hg and ^{129}Xe from Refs. [5,24] are given for comparison.

	^{223}Ra	^{225}Ra	^{223}Rn	^{229}Pa	^{199}Hg	^{129}Xe
α (10^7 η)	2	6	2	60		
ΔE (keV)	50.2	55.2	130.[a]	0.22		
$S_{\rm intr}$ [e fm^3]	22	29	22	28		
S (10^8 $\eta\, e$ fm^3)	500	1100	700	3×10^5	-1.4	1.75
d(at) (10^{25} $\eta\, e$ cm)	3500	7900	1500	3×10^5	5.6	0.47

[a]Calculated.

are in the range $(2-20) \times 10^{-6} \eta\ e\,\text{fm}^3$. This is about 2 orders of magnitude larger than the largest single-particle estimate of $4 \times 10^{-8} \eta\ e\,\text{fm}^3$ given in Ref. [4] for ^{237}Np.

Since the electronic structure of Ra is similar to that of Hg and Rn is similar to Xe, we can use results of atomic calculations for Hg, Xe [5,24] and write

$$d_{\rm at}({\rm Ra}) = d_{\rm at}({\rm Hg}) \frac{(SZ^2R_{1/2})_{\rm Ra}}{(SZ^2R_{1/2})_{\rm Hg}},$$
$$d_{\rm at}({\rm Rn}) = d_{\rm at}({\rm Xe}) \frac{(SZ^2R_{1/2})_{\rm Rn}}{(SZ^2R_{1/2})_{\rm Xe}}, \qquad (31)$$

where we have taken into account the Z dependence of the Schiff moment contribution to the atomic EDM $d_{\rm at}$ due to the increase of electronic wave functions near the nucleus [4] $d_{\rm at} \sim SZ^2R_{1/2}$. The relativistic factor is given by

$$R_{1/2} = \frac{4\gamma_{1/2}}{[\Gamma(2\gamma_{1/2}+1)]^2}\left(\frac{2ZR_0}{a_B}\right)^{2\gamma_{1/2}-2}, \qquad (32)$$

where $\gamma_{1/2} = [1-(Z\alpha)^2]^{1/2}$, a_B is the Bohr radius, and R_0 is the nuclear radius.

We made an estimate also for ^{229}Pa which has the smallest energy splitting between members of g.s. parity doublet among the known octupole deformed nuclei [8]. We assumed the same atomic physics parameters as for Ra, Rn. As seen in Table I the EDM of Ra and Rn are 10^2–10^3 times larger than the EDM of Hg and Xe. We should stress that the phenomenon described in our work occurs probably in many other nuclei that possess octupole deformation (for example, in the Ba-Sm region) and which might be more suitable choice for experimental studies. Experiments with atoms or molecules containing these nuclei may improve substantially the limits on time reversal violation.

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