Enhanced nuclear Schiff moment and time-reversal violation in ^{229}Th-containing molecules

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Octupole deformation results in a strongly enhanced collective Schiff moment in ^{229}Th nucleus. An additional enhancement of time-reversal (T) and parity- (P) violating effects (such as T,P-violating electric dipole moments) appears in the ground $^1\Sigma$ state and in the metastable $^3\Delta_1$ state of diatomic molecule ^{229}ThO. Similar enhancements exist in molecular ions ^{229}ThOH$^+$, ^{229}ThF$^+$, and ^{225,223}RaOH$^+$. Corresponding experiments may be used to test charge conjugation and parity (CP)-violation theories predicting T,P-violating nuclear forces and to search for axions.

I. INTRODUCTION: OCTUPOLE DEFORMATION AND ENHANCED NUCLEAR SCHIFF MOMENTS

Measurements of time-reversal- and parity- (T,P-) and charge conjugation and parity (CP)-violating electric dipole moments (EDM) of elementary particles, nuclei, and atoms provide crucial tests of unification theories and have already cornered many popular models of CP violation, including supersymmetry [1,2]. Corresponding effects are very small; therefore, we are looking for the enhancement mechanisms; see, e.g., Refs. [3–5]. In the present paper it is shown that a strong enhancement can be achieved in the case of atoms and molecules containing ^{229}Th nucleus.

According to the Schiff theorem, nuclear EDM is completely screened in neutral atoms [6]. EDM of diamagnetic atoms is produced by interaction of electrons with nuclear Schiff moment. Schiff moment is a vector multipole which produces an electric field inside a nucleus. It appears in the third order of the multipole expansion of the nuclear electrostatic potential with an added electron screening term [7–11]. Distribution of the Schiff moment electric field inside nucleus, Hamiltonian describing interaction of the Schiff moment with relativistic atomic electrons, and finite nuclear size corrections to the formula for the Schiff moment have been considered in Ref. [12].

References [7,8] calculated the Schiff moment due to proton EDM. References [9–11] calculated (and named) a nuclear Schiff moment produced by the P,T-odd nuclear forces. It was shown in Ref. [9] that contribution of the P,T-odd forces to the nuclear EDM and Schiff moment is ∼40 times larger than the contribution of the nucleon EDM.

Further enhancement of the nuclear Schiff moment may be due to close nuclear levels of opposite parity with the same angular momentum which can be mixed by the T,P-odd nuclear forces [9] (nuclear EDM and magnetic quadrupole

can also be enhanced [13]). Nuclear T,P-odd moments such as magnetic quadrupoles may also be enhanced due to their collective nature in deformed nuclei [14]. However, the largest enhancement (∼10^2–10^3 times) happens in nuclei with octupole deformation where both the close nuclear level effect and the collective effect work together [15,16].

II. CALCULATION OF COLLECTIVE SCHIFF MOMENT

Schiff moment is defined by the following expression [9]:

$$\mathbf{S} = \frac{e}{10}\left[\langle r^2\mathbf{r}\rangle - \frac{5}{3Z}\langle r^2\rangle\langle\mathbf{r}\rangle\right], \qquad (1)$$

where $\langle r^n\rangle \equiv \int \rho(\mathbf{r})r^n d^3r$ are the moments of the nuclear charge density ρ. The second term originates from the electron screening and contains nuclear mean-squared charge radius $\langle r^2\rangle/Z$ and nuclear EDM $d = e\langle\mathbf{r}\rangle$, where Z is the nuclear charge.

If a nucleus has an octupole deformation β_3 and a quadrupole deformation β_2, in the fixed-body (rotating) frame the Schiff moment S_{intr} is proportional to the octupole moment O_{intr}, i.e., it has a collective nature [15,16]:

$$S_{\text{intr}} \approx \frac{3}{5\sqrt{35}}O_{\text{intr}}\beta_2 \approx \frac{3}{20\pi\sqrt{35}}eZR^3\beta_2\beta_3, \qquad (2)$$

where R is the nuclear radius. However, in the laboratory frame EDM and Schiff moment are forbidden by the parity and time-reversal invariance. Indeed, EDM and Schiff moment are polar T-even vectors which must be directed along the nuclear spin I which is a T-odd pseudovector.

Nucleus with an octupole deformation and nonzero nucleon angular momentum has a doublet of close opposite-parity rotational states $|I^\pm\rangle$ with the same angular momentum I ($|I^\pm\rangle = \frac{1}{\sqrt{2}}(|\Omega\rangle \pm |-\Omega\rangle)$), where Ω is the projection of I on to the nuclear axis). The states of of this doublet are mixed by P,T-violating interaction W. The mixing coefficient is

$$\alpha = \frac{\langle I^-|W|I^+\rangle}{E_+ - E_-}. \qquad (3)$$

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This mixing polarizes the nuclear axis **n** along the nuclear spin **I**, $\langle n_z \rangle = 2\alpha \frac{I_z}{I+1}$, and the intrinsic Schiff moment shows up in the laboratory frame [15,16]:

$$S = 2\alpha \frac{I}{I+1} S_{\text{intr}}. \quad (4)$$

Nucleus with an octupole deformation also has a small intrinsic EDM D due to a difference between the proton and neutron distributions which results in the laboratory frame nuclear EDM $d = 2\alpha \frac{I}{I+1} D$ [15,16].[1]

In Refs. [15,16] numerical calculations of the Schiff moments and estimates of atomic EDM produced by the electrostatic interaction between electrons and these moments have been done for ^{223}Ra, ^{225}Ra, ^{223}Rn, ^{221}Fr, ^{223}Fr, ^{225}Ac, and ^{229}Pa. The Schiff moment of ^{225}Ra exceeds the Schiff moment of ^{199}Hg (where the most accurate measurements of the Schiff moment have been performed [18]) 200 times. Even larger enhancement of the ^{225}Ra Schiff moment has been obtained in Ref. [19]. For other nuclei the enhancement factors relative to Hg are between 30 and 700. Atomic relativistic many-body calculations of EDM induced by the Schiff moments in Hg, Xe, Rn, Ra, and Pu atoms have been performed in Refs. [9,20–23] and include additional atomic enhancement mechanisms.

It is useful to make an analytical estimate of the Schiff moment in nuclei with an octupole deformation. According to Ref. [16] the T,P-violating matrix element is approximately equal to

$$\langle I^- | W | I^+ \rangle \approx \frac{\beta_3 \eta}{A^{1/3}} \text{ eV}. \quad (5)$$

Here η is the dimensionless strength constant of the nuclear T,P-violating potential W:

$$W = \frac{G}{\sqrt{2}} \frac{\eta}{2m} (\sigma \nabla) \rho, \quad (6)$$

where G is the Fermi constant, m is the nucleon mass, and ρ is the nuclear number density. Eqs. (2)–(5) give analytical estimate for the Schiff moment:

$$S \approx 1 \times 10^{-4} \frac{I}{I+1} \beta_2 \beta_3^2 Z A^{2/3} \frac{\text{KeV}}{E_- - E_+} e \eta \text{ fm}^3, \quad (7)$$

This estimate gives $S = 280 \, e \, \eta \, \text{fm}^3$ for ^{225}Ra, which is very close to the result of the numerical calculation in Ref. [16] $S = 300 \, e \, \eta \, \text{fm}^3$.

Values of the Schiff moments for nuclei with octupole deformation listed above vary from 45 to 1000 $10^{-8} e\eta$ fm^3

[16]. For spherical nuclei ^{199}Hg, ^{129}Xe, ^{203}Tl, and ^{205}Tl, where the Schiff moment measurements have been performed, calculations [9–11] give the Schiff moment $S \sim 1 \times 10^{-8} \, e\eta \, \text{fm}^3$.

The Schiff moment in Eq. (7) is proportional to the squared octupole deformation parameter β_3^2 which is about $(0.1)^2$. According to Ref. [24], in nuclei with a soft octupole vibration mode the squared dynamical octupole deformation $\langle \beta_3^2 \rangle \sim (0.1)^2$, i.e., it is the same as the static octupole deformation. This means that a similar enhancement of the Schiff moment may be due to the dynamical octupole effect [24–26] in nuclei where $\langle \beta_3 \rangle = 0$.

Unfortunately, the nuclei with the octupole deformation and nonzero spin have a short lifetime. Several experimental groups have considered experiments with ^{225}Ra and ^{223}Rn. The only published EDM measurements [27,28] have been done for ^{225}Ra which has a 15-d half-life. In spite of the Schiff moment enhancement, the ^{225}Ra EDM measurement has not reached yet the sensitivity to the T,P-odd interaction of Eq. (6) comparable to the Hg EDM experiment [18]. The experiments continue; however, the instability of ^{225}Ra and a relatively small number of atoms available may be a problem.

To have a breakthrough in the sensitivity one needs a more stable nucleus and a larger number of atoms. An excellent candidate is the ^{229}Th nucleus, which lives 7917 years and is very well studied in numerous experiments and calculations (this nucleus is the only candidate for the nuclear clock which is expected to have a precision significantly better than atomic clocks [29,30], has strongly enhanced effects of "new physics" [31,32], and may be used for a nuclear laser [33]). ^{229}Th is produced in macroscopic quantities by the decay of ^{233}U (see, e.g., Ref. [34]), and its principal use is for the production of the medical isotopes ^{225}Ac and ^{213}Bi.

According to Ref. [35], ^{229}Th nucleus has octupole deformation with the parameters $\beta_3 = 0.115$, $\beta_2 = 0.240$, $I = 5/2$ and the interval between the opposite-parity levels $E(5/2^-)$–$E(5/2^+) = 133.3$ KeV. The analytical formula in Eq. (7) allows us to scale the value of the Schiff moment from the numerical calculations for ^{225}Ra which has $\beta_3 = 0.099$, $\beta_2 = 0.129$, $I = 1/2$ and the interval between the opposite-parity levels $E(1/2^-)$–$E(1/2^+) = 55.2$ KeV [16]. Then Eq. (7) gives:

$$S(^{229}\text{Th}) = 2 \, S(^{225}\text{Ra}). \quad (8)$$

Using $S(^{225}\text{Ra}) = 300 \times 10^{-8} \, e\eta \, \text{fm}^3$ [16] one obtains $S(^{229}\text{Th}) = 600 \times 10^{-8} \, e\eta \, \text{fm}^3$.

Within the meson exchange theory the π-meson exchange gives the dominating contribution to the T,P-violating nuclear forces [9]. According to Ref. [36] the neutron and proton constants in the T,P-odd potential (6) may be presented as $\eta_n \approx -\eta_p \approx 5 \times 10^6 (-0.2 g \bar{g}_0 + g \bar{g}_1 + 0.4 g \bar{g}_2)$. In Refs. [15,16] we have not separated the proton and neutron contributions. The majority of the nucleons are neutrons, so it make sense to take $\eta = \eta_n$. However, the proton interaction constant has an opposite sign and may cancel a part of the neutron contribution, so we multiply the interaction constant by $[(N - Z)/N] = 0.36$ and use $\eta = 0.36\eta_n$. This way one

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[1] A similar Ω-doublet mixing mechanism produces huge enhancement of electron EDM d_e and T,P-odd interactions in polar molecules, such as ThO. Interaction of d_e with molecular electric field produces the mixing coefficient α, resulting in the orientation of large intrinsic molecular EDM $D \sim ea_B$ along the molecular angular momentum **J**, and we obtain $d = 2\alpha \frac{J}{J+1} D \sim \alpha ea_B$ [17], where a_B is the Bohr radius. As a result, the T,P-violating molecular EDM d exceeds electron EDM d_e by 10 orders of magnitude.

can obtain a rough estimate: $S(^{225}\text{Ra}) = (-2.2g\bar{g}_0 + 11g\bar{g}_1 + 4g\bar{g}_2) e\,\text{fm}^3$, $S(^{229}\text{Th}) = (-4.4g\bar{g}_0 + 22g\bar{g}_1 + 8g\bar{g}_2) e\,\text{fm}^3$.

A more accurate job has been done in Ref. [19] where they presented the Schiff moment as $S(^{225}\text{Ra}) = (a_0 g\bar{g}_0 + a_1 g\bar{g}_1 + a_2 g\bar{g}_2)e\,\text{fm}^3$. To estimate the error, the authors of Ref. [19] have done the calculations using four different models of the strong interaction. They obtained the following sets of the coefficients: $a_0 = -1.5, -1.0, -4.7, -3.0$; $a_1 = 6.0, 7.0, 21.5, 16.9$; $a_2 = -4.0, -3.9, -11.0, -8.8$. Taking the average values of the coefficients and using Eq. (8) gives:

$$S(^{225}\text{Ra}) = (-2.6g\bar{g}_0 + 12.9g\bar{g}_1 - 6.9g\bar{g}_2) e\,\text{fm}^3, \qquad (9)$$

$$S(^{229}\text{Th}) = (-5.1g\bar{g}_0 + 25.7g\bar{g}_1 - 13.9g\bar{g}_2) e\,\text{fm}^3. \qquad (10)$$

These expressions will be used as the final values for the Ra and Th Schiff moments. One can express the results in terms of more fundamental parameters such as the QCD θ-term constant $\bar{\theta}$ and the quark chromo-EDMs $\tilde{d}_u$ and $\tilde{d}_d$ using the relations $g\bar{g}_0 = -0.37\bar{\theta}$ [37] and $g\bar{g}_0 = 0.8 \times 10^{15}(\tilde{d}_u + \tilde{d}_d)/\text{cm}$, $g\bar{g}_1 = 4 \times 10^{15}(\tilde{d}_u - \tilde{d}_d)/\text{cm}$ [1]:

$$S(^{225}\text{Ra}) = 1.0\,\bar{\theta}\,e\,\text{fm}^3, \qquad (11)$$

$$S(^{229}\text{Th}) = 2.0\,\bar{\theta}\,e\,\text{fm}^3, \qquad (12)$$

$$S(^{225}\text{Ra}) = 10^4(0.50\,\tilde{d}_u - 0.54\,\tilde{d}_d)\,e\,\text{fm}^2, \qquad (13)$$

$$S(^{229}\text{Th}) = 10^4(1.0\,\tilde{d}_u - 1.1\,\tilde{d}_d)\,e\,\text{fm}^2. \qquad (14)$$

Note that the contributions of $\bar{\theta}$ and $\tilde{d}_{u,d}$ should not be added to avoid double counting since $\tilde{d}_{u,d}$ may be induced by $\bar{\theta}$.

III. MOLECULAR ENHANCEMENT

Atomic EDM d_a produced by the Schiff moment S very rapidly increases with the nuclear charge Z [3,4,9,16]:

$$d_a \propto Z^2 \left(\frac{a_B}{2ZR}\right)^{2-2\gamma} S, \qquad (15)$$

where R is the nuclear radius, a_B is the Bohr radius, and $\gamma = \sqrt{1 - (Z\alpha)^2}$. Th and Ra have close nuclear charges, $Z = 88$ and 90, and similar electronic structure up to the last filled $7s^2$ subshell. Two extra $6d^2$ electrons in Th have high angular momenta, do not penetrate the nucleus, and do not interact with the Schiff moment directly (up to many-body corrections). Therefore, the d_a/S for Th is approximately equal to the d_a/S for Ra. Using calculations of Ra atom EDM from Refs. [22,23] one can obtain the following estimate:

$$d_a(\text{Th}) \approx -9 \times 10^{-17} \frac{S}{|e|\,\text{fm}^3}\,|e|\,\text{cm} = -2 \times 10^{-16}\bar{\theta}\,|e|\,\text{cm}. \qquad (16)$$

The $d_a(\text{Th})$ as a function of other T,P- and CP-violating interaction constants η, $\bar{g}$, $\tilde{d}$ can be found by the substitution of the Th Schiff moment from the equations in the nuclear Schiff moment section above. This value of Th EDM is three orders of magnitude larger than Hg EDM and four orders of magnitude larger than Xe EDM. However, the Th atom has

nonzero electron angular momentum, $J = 2$, and this reduces the signal coherence time and increases systematic errors. In principle, one may use the Th^{4+} ion, which has closed shells, or look for zero electron angular momentum Th ions in solid-state materials.

Note that the measurements of the effects produced by the ^{229}Th Schiff moment may be used to search for axions. Indeed, the axion dark matter produces oscillating neutron EDM [38] and oscillating Schiff moment [39]; the latter is enhanced in ^{229}Th by the same octupole mechanism. Indeed, the axion dark-matter field $a(t) = a_0\cos(m_a t)$ (m_a is the axion mass) generates oscillating nuclear forces which are similar to the T,P-odd nuclear forces producing the Schiff moments. To obtain the result for the oscillating Schiff moments and EDM it is sufficient to replace the constant $\bar{\theta}$ by $a(t)/f_a$, where f_a is the axion decay constant [38,39]. The search for the effects produced by the oscillating axion-induced Schiff moments in solid-state materials is in progress [40]. A promising direction here may be to use ^{229}ThO molecule placed in a matrix of Xe (or other) atoms. A proposal to use paramagnetic molecules in the matrix of rare-gas atoms for the electron EDM search has been described in Ref. [41].

Promising objects for the Th Schiff moment measurement may be the ThO molecule and the ThOH^+ molecular ion. Both molecules have zero electron angular momentum in the ground state and very close opposite-parity levels which enhance T,P-violating EDM.

Use of polar diatomic molecules for the measurement of the nuclear Schiff moment was suggested in Refs. [7,8] because the electric field inside the polarized molecule exceeds the external electric field ϵ by several orders of magnitude and has the same direction. The molecular polarization is $P \sim D\epsilon/(E_- - E_+)$, where $D \sim ea_B$ is the intrinsic electric dipole moment of the polar molecule. Therefore, to have a significant polarization degree P the interval between the opposite-parity molecular rotational levels $(E_- - E_+)$ should be sufficiently small. Indeed, the rotational interval in molecules is three to five orders of magnitude smaller than a typical interval between the opposite-parity levels in atoms.[2] The experiment has been performed with the TlF molecule [42]. In Ref. [43] it was proposed to study molecule ^{225}RaO, where the effect may be 500 times larger than in TlF due to the enhanced Schiff moment and larger nuclear charge Z. The best sensitivity to the electron EDM has been obtained using molecules ThO [44] and HfF^+ [45] in the excited metastable electronic state $^3\Delta_1$ which contains doublets of very close opposite-parity levels. Finally, in Ref. [46] it was suggested that linear molecules MOH, molecular ions MOH^+ (M is a heavy atom, e.g., Ra in the molecule RaOH^+), and symmetric top molecules (such as MCH_3 or MOCH_3) may be better

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[2]One may interpret molecular enhancement in a different way [17]: Interaction between the Schiff moment and electrons mixes close opposite-parity levels in the molecule, polarizes the molecule along its angular momentum, and creates T,P-violating EDM proportional to the large intrinsic electric dipole moment D; see the discussion below Eq. (4). This enhanced EDM interacts with the external electric field ϵ.

systems than molecules MO since such polyatomic molecules have a doublet of close opposite-parity energy levels in the bending mode and may be polarized by a weak electric field. The reduction of the strength of the necessary electric field simplifies the experiment and dramatically reduces systematic effects.

The T,P-violating effect in ^{229}ThO is much larger than in TlF due to the enhanced Schiff moment and larger nuclear charge. An additional advantage may appear in ThOH$^+$ which is expected to have very close opposite-parity states (similarly to RaOH$^+$). Another possibility may be to use the doublet in $^3\Delta_1$ metastable state of ^{229}ThO (used to improve the limit on electron EDM) and the ground-state doublet $^3\Delta_1$ in ThF$^+$.

The interaction constant W_S for the effective T,P-violating interaction in molecules

$$W_{T,P} = W_S \frac{S}{I} \mathbf{I} \cdot \mathbf{n} \qquad (17)$$

(here $\mathbf{I}$ is the nuclear spin, $\mathbf{n}$ is the unit vector along the molecular axis) in ThO, ThOH$^+$, and RaOH$^+$ may be estimated by the comparison with the RaO molecule. Calculation of W_S for RaO has been done in Ref. [47]: $W_S(\text{RaO}) = 45\,192$ atomic units (here a.u. $= e/a_B^4$).

In the RaOH$^+$ ion the electron density on the Ra nucleus is slightly smaller than in RaO (since a part of the electron charge density moves to hydrogen); therefore, one can assume $W_S(\text{RaOH}^+) \approx 30\,000$ a.u. In ThO and in ThOH$^+$ electron density on the Th nucleus is expected to be slightly larger than that for Ra due to the higher Th charge and two extra electrons. Therefore, one can assume $W_S(\text{ThO}) \approx 50\,000$ a.u. and $W_S(\text{ThOH}^+) \approx 30\,000$ a.u. Note that the electron wave function in the bending molecular mode of RaOH$^+$ and ThOH$^+$ is the same as in their ground states; therefore, the parameters W_S are practically not affected by these bending vibrations (where there is the doublet of the opposite-parity levels). Parameter W_S in the $^3\Delta_1$ state of the ^{229}ThO molecule should have comparable value to their ground-state values since $^3\Delta_1$ and the ground $^1\Sigma_0$ state differ by one electron orbital only. The $^3\Delta_1$ state in the ThF$^+$ molecular ion is similar to the $^3\Delta_1$ state in the ^{229}ThO molecule.

The estimates presented above are based on comparison with the numerical calculations of the Schiff moment contribution in RaO. Estimates based on the Z dependence extrapolation Eq. (15) from TlF give 2 times larger results.

Substitution of the Schiff moment (12) to the energy shift $W_{T,P} = W_S \frac{S}{I} \mathbf{I} \cdot \mathbf{n}$ gives for the fully polarized molecule the energy difference between the $I_z = I$ and $I_z = -I$ states in ^{229}ThO:

$$2W_S S = 1 \times 10^7 \bar{\theta} \, h \, \text{Hz}, \qquad (18)$$

where h is the Plank constant. A similar estimate is valid for molecular ions ThF$^+$ and ThOH$^+$. The measured shift in the 1991 TlF experiment [42] was -0.13 ± 0.22 mHz. The same sensitivity in the ^{229}ThO, ThF$^+$, or ThOH$^+$ experiments would allow one to improve the current limit $|\bar{\theta}| < 10^{-10}$ and also the limits on other fundamental parameters of the CP-violation theories such as the strength of T,P-violating potential η, the πNN interaction constants $\bar{g}$, and the quark chromo-EDMs $\tilde{d}$.

IV. COMPARISON WITH EXISTING AND PROPOSED EXPERIMENTS

We should compare the suggested experiments with the ^{229}ThO, ThF$^+$, and ^{229}ThOH$^+$ molecules with other existing and proposed experiments. The best limit on the nuclear Schiff moment has been obtained in the measurement of Hg EDM [18]. However, there is a theoretical problem here: The most recent sophisticated calculation [48] was not able to find out even the sign of the Hg Schiff moment, and different interaction models give very different results. There are two reasons for this: First, the Schiff moment is determined by the charge distribution of the protons. However, it is directed along the nuclear spin which in ^{199}Hg is carried by the valence neutron, i.e., the Schiff moment in ^{199}Hg is determined by the many-body effects, which are harder to calculate. The second reason is in the formula for the Schiff moment defined by Eq. (1). There are two terms of opposite sign in this formula which tend to cancel each other, the main term and the screening term (note that the screening term kills the nuclear EDM contribution to the atomic EDM). If we do not know each term sufficiently accurately, then the final sign and the magnitude of the Schiff moment are unknown.

Recently, interest in EDM experiments has moved toward molecules where the effects are very strongly enhanced by the close rotational levels and very strong internal "effective electric field." For example, the limit on electron EDM in ThO and HgF$^+$ experiments have been improved by more than an order of magnitude in comparison with the atomic EDM experiments. The Tl nuclear Schiff moment has been measured in the TlF experiment [42]. Similarly to ^{199}Hg, calculations of the ^{203,205}Tl Schiff moments suffer from the problem of the cancellation between two approximately equal terms in Eq. (1) and the problem of the nuclear core polarization contribution (since there is a strong cancellation between the two terms in the valence proton contribution in Tl [9,11,36]).

Actually, the interpretation of the TlF experiment [42] was done in terms of the proton EDM. However, here we probably have a more serious problem (below we will follow the discussion in Ref. [36]). First, calculations with different choices of the strong interaction give different signs and magnitudes of the Schiff moment S_p induced by the proton EDM (since we also have here the cancellation between the main and the screening contributions). The authors of the molecular calculation in Ref. [49] selected the maximal value of four numbers calculated by A. Brown (this maximal number leads to the strongest limit on the proton EDM), and this value of S_p was used in all other molecular calculations for TlF [50–52] (see also Ref. [22]). There was no such accuracy investigation for the proton EDM contribution to the Hg Schiff moment, but naively we may expect that the accuracy is actually lower than in Tl since the valence nucleon in ^{199}Hg is a neutron.

The second problem is that in practically any model the contribution of the T,P-violating nuclear forces to the Schiff moment is one to two orders magnitude larger than the proton EDM contribution (the ratio is "model independent" since the πNN interaction constant appears in both contributions and cancels out in the ratio). Therefore, to obtain the limit on the proton EDM, we neglect the much larger contribution of the

P,T-odd nuclear forces. Thus, in the Particle Data tables the limit on the proton EDM is presented assuming that there are no other contributions to atomic and molecular EDM. However, if we wish to test CP-violation theories, then such limits on the proton EDM from Hg and Tl EDM can hardly be used.

These theoretical problems do not exist for the collective Schiff moments in the nuclei with the octupole deformation. The second screening term is very small in this case since it is proportional to a very small intrinsic dipole moment D of the "frozen" nucleus. If the distributions of the neutrons and protons are the same, $D = 0$. Thus, there is no cancellation and the intrinsic Schiff moment is proportional to the known electric octupole moment (which may actually be measured using probabilities of the octupole transitions between the rotational levels). Then the calculation is reduced to the expectation value of the T,P-odd interaction $\langle \Omega | W | \Omega \rangle$, here $|\Omega\rangle$ is the ground state of the "frozen" deformed nucleus [15,16]. Calculation of one expectation value looks more reliable than the calculation of the infinite sum $\sum_n \frac{|n\rangle\langle n|W|0\rangle}{E_0 - E_n}$ in nuclei where there is no single dominating contribution. Thus, calculations of the collective Schiff moments look more "clean" theoretically. More importantly, the collective Schiff moment is enhanced by two to three orders of magnitude.

V. CONCLUSION

In the present paper it is proposed to search for the T,P- and CP-violating effects in the molecule ^{229}ThO where the effects are two to three orders of magnitude larger than in TlF due to the enahnced Schiff moment of the ^{229}Th nucleus and large nuclear charge. An additional advantage may be in the ^{229}ThOH$^+$ molecular ion, in the $^3\Delta_1$ state of the ^{229}ThO molecule, and in the ^{229}ThF$^+$ molecular ion, which have very close opposite-parity energy levels and may be polarized by a weak electric field. The $^3\Delta_1$ state of the ^{229}ThO molecule has already been used to measure electron EDM. The enhanced effects in these molecules may also be used to search for axions. ^{229}Th lives 7917 years, may be produced in macroscopic quantities (as it is done for the medical applications), and is very well studied in numerous experiments.

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