Enhanced *T*-odd, *P*-odd electromagnetic moments in reflection asymmetric nuclei

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Collective P- and T-odd moments produced by parity and time invariance violating forces in reflection asymmetric nuclei are considered. The enhanced collective Schiff, electric dipole, and octupole moments appear due to the mixing of rotational levels of opposite parity. These moments can exceed single-particle moments by more than 2 orders of magnitude. The enhancement is due to the collective nature of the intrinsic moments and the small energy separation between members of parity doublets. In turn these nuclear moments induce enhanced T- and P-odd effects in atoms and molecules. A simple estimate is given and a detailed theoretical treatment of the collective T-, P-odd electric moments in reflection asymmetric, odd-mass nuclei is presented. In the present work we improve on the simple liquid drop model by evaluating the Strutinsky shell correction and include corrections due to pairing. Calculations are performed for octupole deformed long-lived odd-mass isotopes of Rn, Fr, Ra, Ac, and Pa and the corresponding atoms. Experiments with such atoms may improve substantially the limits on time reversal violation. [S0556-2813(97)00809-1]

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I. INTRODUCTION

In 1964 Christenson *et al.* [1] discovered that CP is violated in the decay of neutral K mesons. As one expects the CPT theorem to be valid this discovery implied that time reversal (T) is violated in the observed decays of the kaon. This fact immediately led to the search for CP or T violation in other systems. Since the 1960s many attempts have been made to observe T violation in systems different from the kaons. Time reversal violation has not been observed so far but upper limits for T conservation have been established. The search for time reversal violation encompasses a large variety of physical systems and involves many methods. One of the more widely used methods involves the search for static T-, P-odd electromagnetic moments, moments that would be absent if the Hamiltonian of the system is even under time reversal and reflection. Such moments include the electric dipole moment (EDM), the electric octupole, the magnetic quadrupole, etc. Early on, with the discovery of CP violation, attempts were made to measure the electric dipole moment of the neutron and at present significant upper limits depend on the existence of such moment [2,3]. The neutron was not the only system in which attempts were made to find a static electric dipole moment. Experiments with atoms and molecules were performed in which upper limits for electric dipole moments of the respective systems were established. In fact the recent measurements of dipole moments of Hg and Xe atoms [4] and TlF molecule [5] have established upper limits for time reversal violating nucleon-nucleon and quark-quark interactions that are of the same order (or maybe even exceed) the limits obtained in the measurement of the neutron dipole moment.

The existence of a static atomic dipole moment may be due to the following three reasons: (a) the possible existence of a dipole moment of the electron (the best limits on the electron EDM were obtained in Tl atom EDM measurements in Ref. [6], see also Cs measurements in Ref. [7]); (b) time reversal violation in the electron-nucleon interaction, thus in the lepton-hadron interactions; (c) the possible existence of a static T-odd, P-odd moment of the nucleus arising from the time reversal violating component of the hadron-hadron interactions. The recent experiments with Hg gave the best limit on this interaction. This possibility will also be the subject of this work.

In a recent paper [8] we put forward a suggestion that rotating nuclei that have static octupole deformations when viewed in their intrinsic (body) frame of reference will have enhanced T-odd, P-odd (for short T-, P-odd) moments if a time reversal and parity violating interaction is present in the nuclear Hamiltonian. In the intrinsic frame the nucleus with an octupole deformation has large octupole, Schiff, and dipole moments. An orientation of these moments is connected to a nuclear axis $\boldsymbol{n}$ (e.g., the dipole moment is $\boldsymbol{d}=d\boldsymbol{n}$). In a stationary rotational state the mean orientation of the axis vanishes ($\langle \boldsymbol{n}\rangle=0$) since the only possible correlation $\langle \boldsymbol{n}\rangle \propto \boldsymbol{I}$ violates time reversal invariance and parity (here $\boldsymbol{I}$ is the total angular momentum of the system). Therefore, the mean values of electric dipole, octupole and Schiff moments vanish in laboratory frame if there is no T, P violation. In the nuclei with the octupole deformation and nonzero intrinsic angular momentum there are doublets of rotational states of opposite parity with the same angular momentum $\boldsymbol{I}$ (in molecular physics this phenomenon is called Λ doubling). A T-, P-odd interaction mixes these rotational levels. As a result the nuclear axis becomes oriented along the total angular momentum, $\langle \boldsymbol{n}\rangle \propto \alpha \boldsymbol{I}$ where α is the mixing coefficient. Due to this orientation of the nuclear axis by a T-, P-odd interaction the mean values of the T-, P-odd moments are not zero in the laboratory frame, e.g., $\langle \boldsymbol{d}\rangle = d\langle \boldsymbol{n}\rangle \propto \alpha d \boldsymbol{I}$.

We find two basic enhancement factors in this mechanism: first, in the intrinsic frame the nucleus with an octupole deformation will have large octupole, Schiff, or dipole electric moments because a large number of nucleons will contribute to the moments, and second due to the appearance of closely spaced parity doublets in the spectrum of the nucleus with octupole deformation. It is not only that the spacing between the members of the doublets is small but also (T-, P-odd) interaction will mix well two such states. The enhanced nuclear Schiff moments that result in such nucleus with a reflection asymmetric shape will induce ~1000 times enhanced atomic electric dipoles, and measurements performed with such atoms may improve upper limits for time reversal violation.

It is the aim of the present work to examine in detail the consequences of the intrinsic reflection asymmetry on the T-, P-odd electromagnetic moments in nuclei produced by T-, P-odd components in the nuclear force and on the induced T-, P-odd moments in the corresponding atoms. In this paper we extend the work in Ref. [8] attempting to provide an improved and more detailed theory of the nuclei with asymmetric shapes and of the resulting T-, P-odd moments if parity time reversal is violated to some degree in the nuclear force.

Present experimental studies of nuclei in the actinide region (Z around 88 and N around 134) indicate that these nuclei possess octupole shapes in the ground state (g.s.) [9–12]. In these nuclei near the Fermi energy, orbital pairs are coupled strongly by the octupole-octupole part of the effective nuclear interaction. The existence of octupole deformations in the actinide nuclei is manifested in the existence of parity doublet states and parity doublet bands. The $E1$ and $E3$ transitions between these states are relatively strong, of the order of a Weisskopf unit. These experimental findings are supported by theoretical studies. Some isotopes of Rn, Fr, Ra, Ac, Th, and Pa in the $218<A<230$ region are predicted theoretically to be reflection asymmetric in the g.s. The phenomena of octupole instability are observed and described theoretically also around $Z\sim56$, $N\sim88$. Several isotopes of Ba, Ce, Nd, and Sm in the $A=140–152$ region are known to be octupole-soft and develop reflection asymmetric shapes at higher spins but no experimental data at present can confirm such shapes in the g.s. [11,12]

We will present in this work results for relatively long-lived neutron-odd isotopes of Rn, Ra, and proton-odd isotopes of Fr, Ac, and Pa for which there is theoretical and in most cases experimental evidence of reflection-asymmetric intrinsic shapes in the g.s.

We use the results of the Nilsson-Strutinsky mean field calculations [13] and employ the Leander *et al.* [14] particle plus core model to calculate the wave functions, energy splittings and T-, P-odd interaction matrix elements between members of the parity doublets. In the calculation of the intrinsic dipole, Schiff and octupole electric moments we use a two-liquid drop model. Strutinsky corrections and corrections due to pairing are taken into account in this work.

In the past one conjectured that T-, P-odd moments will be enhanced in the cases when close to the g.s. there is, for whatever reason, a level with the same spin and opposite parity [15–18]. The connection between enhanced $E1$ transitions between these levels and the nuclear electric dipole moment was made in the work of Haxton and Henley [17]. At that time, nuclei which possess an intrinsic reflection asymmetry and quadrupole deformed nuclei without such an asymmetry but in which an accidentally close ''parity doublet'' exists, were treated on an equal footing [17]. The fact that in some nuclei systematically enhanced $E1$ matrix elements are the direct consequence of intrinsic reflection asymmetry was realized and investigated extensively by Leander *et al.* several years later [19].

In the work [18] the Schiff moment induced by nuclear T-, P-odd forces was introduced in the presently used form and calculations for Xe, Hg, Tl, and other interesting cases were done. The calculations of the atomic electric dipole moments induced by the nuclear T-, P-odd Schiff moments were also presented (we should note that similar considerations for T-, P-odd effects in molecules and atoms induced by the proton electric dipole moment were applied in [20,21]).

In our earlier paper [8] the connection was made between the collective T-, P-odd electric moments in the *intrinsic frame* of reference in reflection-asymmetric nuclei and these moments in the *laboratory* frame [24]. Due to the collective nature of the intrinsic moments and the nearly identical intrinsic structure of the parity doublets one expects that the electric T-, P-odd moments will be maximal.

After the present introduction in Sec. II we define the T-, P-odd moments, including the Schiff moment. In Sec. III we present a simple expression for a T-, P-odd moment in the case of a deformed rotating nucleus in the presence of a T-, P-odd interaction. The first part of Sec. IV deals with the calculation of the dipole, Schiff, and octupole intrinsic moments in a two-fluid liquid drop model. In the same section we bring a simple schematic estimate of a Schiff moment in an octupole deformed nucleus. Next we present the particle +core model and describe the calculation of the T-, P-odd matrix elements and mixing amplitudes. In Sec. V the numerical results are presented for each of the nuclei and at the end of this section results are given for the atomic dipole moments. In the last section (Sec. VI) a summary is presented.

II. ATOMIC ELECTRIC DIPOLE AND NUCLEAR *T*-, *P*-ODD MOMENTS

We start from the electrostatic potential of a nucleus screened by the electrons of the atom. If the nucleus has a T-, P-odd dipole moment the dipole term in the potential vanishes in accordance with the Purcell-Ramsey-Schiff theorem [22,23] (see the derivation in the Appendix):

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

Here $\rho(\boldsymbol{r})$ is the nuclear charge density, $\int\rho(\boldsymbol{r})d^3\boldsymbol{r}=Z$, and $\boldsymbol{d}=\int e\boldsymbol{r}\rho(\boldsymbol{r})d^3\boldsymbol{r}$ is the electric dipole moment (EDM) of the nucleus. The first term in this expression is usual electrostatic nuclear potential, and the second term is a result of the electron screening effect. The multipole expansion of $\varphi(\boldsymbol{R})$ contains both T-, P-even and T-, P-odd terms. We consider here only the latter. The dipole part in Eq. (1) is canceled by the second term in this equation:

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

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

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

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 $\boldsymbol{S}$ and a rank 3 tensor $Q_{\alpha\beta\gamma}$ (see, e.g., [18]):

$$\varphi^{(3)}=\varphi^{(3)}_{\text{Schiff}}+\varphi^{(3)}_{\text{octupole}},$$

$$\varphi^{(3)}_{\text{Schiff}}=-\boldsymbol{S}\boldsymbol{\nabla}\Delta\frac{1}{R}=4\pi\boldsymbol{S}\boldsymbol{\nabla}\delta(R),$$

$$\varphi^{(3)}_{\text{octupole}}=-\frac{1}{6}Q_{\alpha\beta\gamma}\nabla_\alpha\nabla_\beta\nabla_\gamma\frac{1}{R}, \tag{4}$$

where

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

is the Schiff moment (SM) and

$$Q_{\alpha\beta\gamma}=\int e\rho(\boldsymbol{r})\left(r_\alpha r_\beta r_\gamma-\frac{1}{5}r^2(\delta_{\alpha\beta}r_\gamma+\delta_{\beta\gamma}r_\alpha+\delta_{\alpha\gamma}r_\beta)\right)d^3\boldsymbol{r},$$

$$Q_{zzz}\equiv\frac{2}{5}Q_3=\frac{2}{5}\sqrt{\frac{4\pi}{7}}\int e\rho(\boldsymbol{r})r^3Y_{30}d^3\boldsymbol{r} \tag{6}$$

is the electric octupole moment. Because the intrinsic dipole moment of the nucleus appears in second order in the nuclear deformation [see Eq. (21)] a correction to the octupole field which arises from the nonspherical part of the density in the screening term in Eqs. (3) and (5) can be neglected. Indeed, this correction is at least third order in the nuclear deformation.

In the absence of T- and P-violating interactions the electric dipole moment of an atom is equal to zero. The interaction between atomic electrons and the T-, P-odd part of the electrostatic nuclear potential in Eq. (4) will mix atomic states of the opposite parity and thus generate an atomic electric dipole moment:

$$D_z=-e\langle\tilde{\psi}|r_z|\tilde{\psi}\rangle=-2e\sum_{|k_2\rangle}\frac{\langle k_1|r_z|k_2\rangle\langle k_1|-e\varphi^{(3)}|k_2\rangle}{E_{k_1}-E_{k_2}}, \tag{7}$$

where $\tilde{\psi}$ denotes the perturbed atomic wave function, $|k_1\rangle=|k_1,J_1,J_{1z}\rangle$ is the unperturbed electron ground state, and $\{|k_2\rangle\}$ is the set of opposite parity states with which $|k_1\rangle$ is mixed due the perturbation $-e\varphi^{(3)}$.

The most accurate measurements of atomic and molecular T-, P-odd electric dipole moments have been done in the atoms Xe and Hg with zero electron angular momentum, $J_1=0$. Examining Eq. (7) it is easy to demonstrate that in such atoms nuclear electric octupole (as well as another T-, P-odd moment, magnetic quadrupole) cannot generate an atomic electric dipole. Indeed, according to the triangle rule for the addition of angular momenta, $\langle k_1|r_z|k_2\rangle$ can only have a nonzero value if $|J_1-J_2|\leqslant 1\leqslant J_1+J_2$. Similarly, for $\langle k_1|\varphi^{(3)}_{\text{octupole}}|k_2\rangle$ to be nonzero, we must have $|J_1-J_2|\leqslant 3\leqslant J_1+J_2$. This implies that the following conditions need to be satisfied for the dipole moment to be nonzero:

$$|J_1-J_2|\leqslant 1 \quad\text{and}\quad J_1+J_2\geqslant 3. \tag{8}$$

The lowest pair of values that satisfies this condition is $J_1=3/2$ and $J_2=3/2$ for the states with one or odd number of electrons outside the closed subshells, and $J_1=1$, $J_2=2$ for states with even number of electrons. In the case of the magnetic quadrupole one needs $J_1+J_2\geqslant 2$, i.e., the lowest pair is $J_1=1/2$, $J_2=3/2$. Hence, the nuclear electric octupole and magnetic quadrupole moments cannot contribute to the atomic electric dipole moment of $J_1=0$ states. Therefore, we mostly center our considerations on the Schiff moment. Note also that the T-, P-odd part of the electrostatic nuclear potential in Eq. (4) is concentrated mainly inside the nucleus. As a result the induced atomic electric dipole moment is proportional to the density of external electrons at the nucleus (more accurately, to the gradient of this density) which rapidly increases with the nuclear charge Z. This is why in general heavy atoms and nuclei are favored in the studies of T-, P-odd moments.

III. T-, P-ODD MOMENTS AND ROTATIONAL DOUBLETS

If a deformed nucleus in the *intrinsic* (body-fixed) frame of reference is reflection asymmetric, it can have collective T-, P-odd moments. As a consequence of this reflection asymmetry, rotational doublets appear in the laboratory system. Without T-, P-violating forces a T-, P-odd moment vanishes exactly in the laboratory. A T-, P-odd interaction however may reveal such intrinsic T-, P-odd moments in the laboratory frame. Consider a nearly degenerate rotational parity doublet in the case of an axially symmetric nucleus. The wave functions of the members of the doublet are written as [24]

$$\Psi^\pm=\frac{1}{\sqrt{2}}(|IMK\rangle\pm|IM-K\rangle). \tag{9}$$

Here $\boldsymbol{I}$ is the nuclear spin, $M=I_z$ and $K=\boldsymbol{I}\boldsymbol{n}$, where $\boldsymbol{n}$ is a unit vector along the nuclear axis.

The *intrinsic* dipole and Schiff moments are directed along $\boldsymbol{n}$:

$$\boldsymbol{d}_{\text{intr}}=d_{\text{intr}}\boldsymbol{n},$$

$$\boldsymbol{S}_{\text{intr}}=S_{\text{intr}}\boldsymbol{n}. \tag{10}$$

For these good parity states $\langle\Psi^\pm|\boldsymbol{I}\boldsymbol{n}|\Psi^\pm\rangle=0$ because K and $-K$ have equal probabilities and this means that there is no average orientation of the nuclear axis in the laboratory frame ($\langle\Psi^\pm|\boldsymbol{n}|\Psi^\pm\rangle=0$). This is a consequence of time invariance and parity conservation since the correlation $\boldsymbol{I}\boldsymbol{n}$ is T-, P-odd. As a result of $\langle\Psi^\pm|\boldsymbol{n}|\Psi^\pm\rangle=0$, the mean value of the T-, P-odd moments (whose orientation is determined by the direction of the nuclear axis) is zero in the laboratory frame.

A T-, P-odd interaction V^{PT} will mix the members of the doublet. The admixed wave function of the predominantly positive parity member of the doublet will be $\Psi=\Psi^{+}+\alpha\Psi^{-}$ or

$$\Psi=\frac{1}{\sqrt{2}}[(1+\alpha)|IMK\rangle+(1-\alpha)|IM-K\rangle], \tag{11}$$

where α is the T-, P-odd admixture

$$\alpha=\frac{\langle\Psi^{-}|V^{PT}|\Psi^{+}\rangle}{E^{+}-E^{-}}, \tag{12}$$

and $E^{+}-E^{-}$ is the energy splitting between the members of the parity doublet. A similar expression is obtained for the negative parity member of the doublet.

In the T-, P-admixed state

$$\langle\Psi|\boldsymbol{In}|\Psi\rangle=\langle\Psi|\hat{K}|\Psi\rangle=2\alpha K, \tag{13}$$

i.e., the nuclear axis $\boldsymbol{n}$ is oriented along the nuclear spin $\boldsymbol{I}$:

$$\langle\Psi|n_z|\Psi\rangle=2\alpha\frac{KM}{(I+1)I}. \tag{14}$$

Therefore in the laboratory system the electric dipole and Schiff moments obtain nonzero average values. For example, in the ground state (g.s.) usually $M=K=I$ and

$$\langle\Psi|S_z|\Psi\rangle=2\alpha\frac{I}{I+1}S_{\text{intr}}. \tag{15}$$

IV. NUCLEAR MODELS OF THE *T*-, *P*-ODD MOMENTS

A. Nuclear shape and intrinsic moments

In this paper we consider the moments of heavy deformed nuclei in the ground states. The main contribution to the electric moments comes from the even-even core which is well described by the two-fluid liquid drop model, see, e.g., Refs. [25,26,24]. The surface of an axially symmetric deformed nucleus is

$$R=c_V(\beta)R_0\left(1+\sum_{l=1}\beta_l Y_{l0}\right), \tag{16}$$

where $c_V=1-(1/\sqrt{4\pi})\Sigma_{l=1}\beta_l^2$ ensures the volume conservation and $R_0=r_0A^{1/3}$. For the sake of brevity and because the nuclear deformations we deal with are relatively small $\beta_2<0.2$, $\beta_{3,4}<0.1$ we will put in our discussion the coefficient $c_V(\beta)=1$. [In the actual calculations R_0 is replaced by $c_V(\beta)R_0$.]

If the nucleus is reflection asymmetric then the β_1 deformation parameter is needed to keep the center of mass fixed at $z=0$, i.e., $\int z d^3\boldsymbol{r}=0$. In lowest order in nuclear deformations [27,28,24]

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

Due to the Coulomb force protons and neutrons are differently distributed over the nuclear volume. From the requirement of a minimum in the energy [25,19]

$$\frac{\rho_p(\boldsymbol{r})-\rho_n(\boldsymbol{r})}{\rho_p(\boldsymbol{r})+\rho_n(\boldsymbol{r})}=-\frac{1}{4C}V_{\text{Coul}}(\boldsymbol{r}), \tag{18}$$

where $\rho_p\equiv\rho$ and ρ_n are the proton and neutron densities, $V_{\text{Coul}}(\boldsymbol{r})$ is the Coulomb potential created by $\rho_p(\boldsymbol{r})$ and C is the volume symmetry-energy coefficient of the liquid drop model. To lowest order [19]

$$\rho=\frac{\rho_0}{2}-\frac{\rho_0}{8}\frac{e^2Z}{CR_0}\left[\frac{3}{2}-\frac{1}{2}\left(\frac{r}{R_0}\right)^2+\sum_{l=1}\frac{3}{2l+1}\left(\frac{r}{R_0}\right)^l\beta_l Y_{l0}\right], \tag{19}$$

where $\rho_0=3A/(4\pi R_0^3)$. The coefficient C is not known very accurately, its value for nuclei studied here is in the range 20–35 MeV [19,28,29]. Note that requiring $\int\rho(\boldsymbol{r})d^3\boldsymbol{r}=Z$ one has in lowest order [25]

$$Z=\frac{1}{2}A\left(1-\frac{3}{10}\frac{e^2Z}{CR_0}\right). \tag{20}$$

We compute the intrinsic Schiff moment by substituting the density in Eq. (19) into Eq. (5). Because of the relative shift of protons versus neutrons the nucleus in the intrinsic frame has a dipole moment as calculated in the past [27,30,19,28] and given by

$$d_{\text{intr}}=eAZ\frac{e^2}{C}\frac{3}{40\pi}\sum_{l=2}\frac{(l^2-1)(8l+9)}{[(2l+1)(2l+3)]^{3/2}}\beta_l\beta_{l+1}. \tag{21}$$

A more detailed treatment of the intrinsic dipole moment includes also the neutron skin effect which reduces d_{intr} somewhat [28,29]. To discuss corrections to the intrinsic SM it is convenient to decompose it into two terms

$$S_{\text{intr}}=S_{\text{intr}}^{(1)}+S_{\text{intr}}^{(2)}. \tag{22}$$

The first term includes only contribution from the constant part of the density, $\rho(r=0)$ in Eq. (19). In lowest order in deformation it equals to

$$S_{\text{intr}}^{(1)}=eAR_0^3\frac{3}{40\pi}\left(1-\frac{e^2Z}{R_0C}\frac{3}{8}\right)\sum_{l=2}\frac{(l+1)\beta_l\beta_{l+1}}{\sqrt{(2l+1)(2l+3)}}. \tag{23}$$

As observed above this contribution comes from the first term in Eq. (5) only. The second term is due to the Coulomb redistribution of the proton density and stems from the last two terms in the brackets in Eq. (19). A simple derivation gives

$$S_{\text{intr}}^{(2)}=eAR_0^3\frac{3}{40\pi}\frac{e^2Z}{R_0C}\frac{29}{280}\sum_{l=2}\frac{(l+1)\beta_l\beta_{l+1}}{\sqrt{(2l+1)(2l+3)}}. \tag{24}$$

This term gives about 10% contribution for nuclei with $Z\sim 90$. Using Eq. (20) one can approximate the intrinsic SM as

$$S_{\rm intr}\simeq eZR_0^3\frac{3}{20\pi}\sum_{l=2}\frac{(l+1)\beta_l\beta_{l+1}}{\sqrt{(2l+1)(2l+3)}}. \tag{25}$$

The contribution of the $\beta_3\beta_4$ term in both $d_{\rm intr}$ and $S_{\rm intr}$, for the nuclei studied here, is of about the same size as the contribution of the $\beta_2\beta_3$ term.

The expression for the intrinsic octupole moment is [24,31]

$$Q_{3\,{\rm intr}}=\frac{3eZR_0^3}{2\sqrt{7\pi}}\left(\beta_3+\frac{2}{3}\sqrt{\frac{5}{\pi}}\beta_2\beta_3+\frac{15}{11\sqrt{\pi}}\beta_3\beta_4+\cdots\right). \tag{26}$$

Various nuclear surface corrections to the density of nucleons such as the neutron skin are not included in the above equations for the SM. For the intrinsic dipole moment these corrections were included in Refs. [28,29] using the droplet model. The corrections for $d_{\rm intr}$ are of the same order as the main term in Eq. (21) but have the opposite sign. One can conclude from Eqs. (21)–(25) that since such corrections alter only the term $S_{\rm intr}^{(2)}$ they can contribute to the Schiff moment at most 10%.

Values of the Schiff moment obtained using Eq. (25) are about 30% less than given by the direct calculation using Eqs. (5) and (19) (with $C\approx 27$ MeV corresponding to the value obtained in the droplet model which includes the effect of a neutron skin [28,29]). This is partly due to terms of higher orders in the deformation not included in Eqs. (20)–(25).

Both the intrinsic SM and dipole moments are second order in nuclear deformation and may turn out to be sensitive to details of the proton density distribution. Because of that it is important to take into account quantum mechanical corrections to the liquid drop model. Such correction can be included through the Strutinsky shell correction method [32,33]. In this method the level density is decomposed into a smooth averaged density and a remaining part, fluctuating with the shell filling. The corrected expectation value of a one-body operator, e.g., the intrinsic Schiff moment (for the similar treatment of the intrinsic dipole moment see Refs. [19,29]) is written as a sum of ''macroscopic'' and shell correction terms [33]

$$\tilde{S}_{\rm intr}=S_{\rm intr}^M+S_{\rm intr}^{\rm shell}. \tag{27}$$

As the ''macroscopic'' part one takes the liquid drop moment, in the case of the Schiff moment $S_{\rm intr}^M$ is given in lowest order in β_i by Eq. (22) or by approximate Eq. (25). The shell correction term is given by [33,19,29]

$$S_{\rm intr}^{\rm shell}=\sum_i (v_i^2-n_i)\langle i|S|i\rangle, \tag{28}$$

where v_i^2 are the BCS quasiparticle occupation numbers and n_i — the smoothed single-particle occupation numbers, for the state i. The latter are determined by the averaged level density and energies of the states i in the single-particle potential. (Detailed expressions can be found in Refs. [33,34].)

It is convenient to express the corrections relatively to the $S_{\rm intr}^M$. The second term in Eq. (5) is proportional to the intrinsic dipole moment $d_{\rm intr}$. The shell correction to $d_{\rm intr}$ was studied in detail in [19,29]. The results show that the shell correction to $d_{\rm intr}$ is of the same order of magnitude as the ''macroscopic'' dipole moment given by Eq. (21). Therefore the subsequent correction to the second term of the intrinsic SM in Eq. (5) does not exceed (5–7)% of the value of $S_{\rm intr}^M$.

The shell correction to the deviation of proton and neutron centers of mass for octupole deformed actinide nuclei was also investigated in Refs. [19,29]. The deviation of the center of mass can be represented formally as a change of the β_1 deformation parameter, because $\int z\rho_t d^3\boldsymbol{r}\sim R_0[\beta_1+\sqrt{(3/4\pi)}(9/\sqrt{35})\beta_2\beta_3+\cdots]$. Note that the intrinsic Schiff moment is in the lowest order proportional to the β_1 for protons [Eqs. (17) and (23)–(25)]. Therefore the resulting shell correction for the first term of the intrinsic SM in Eq. (5) is analogous to the one obtained in [19,29] for the proton center of mass.

B. The P- and T-odd interaction

The P- and T-odd nucleon-nucleon two-body potential can be written in the form [35,36] as

$$W_{ab}=\frac{G}{\sqrt{2}}\frac{1}{2m}[(\eta_{ab}\boldsymbol{\sigma}_a-\eta_{ba}\boldsymbol{\sigma}_b)\boldsymbol{\nabla}_a\delta(\boldsymbol{r}_a-\boldsymbol{r}_b)+\eta'_{ab}[\boldsymbol{\sigma}_a\times\boldsymbol{\sigma}_b]\{(\boldsymbol{p}_a-\boldsymbol{p}_b),\delta(\boldsymbol{r}_a-\boldsymbol{r}_b)\}], \tag{29}$$

where $G=10^{-5}/m^2$ is the Fermi constant (m is the nucleon mass), a,b designate a proton or neutron and the curly brackets denote the anticommutation operation. Note, that η_{ab} are in fact effective constants. In this work we use the corresponding effective one-body P- and T-odd potential [18,36,37]

$$V^{PT}=\frac{G}{\sqrt{2}}\frac{\eta}{2m}\rho_0\sum_i \boldsymbol{\sigma}_i[\boldsymbol{\nabla}_i f(\boldsymbol{r}_i)], \tag{30}$$

where $\rho_t(\boldsymbol{r})=\rho_0 f(\boldsymbol{r})$is the nuclear density. We assume [35,36] that effective constants η_{ab} and η are of the same order in magnitude. For the deformed nuclear density we use the expansion [24]

$$\rho(\boldsymbol{r})=\rho_0(r)-R_0\frac{\partial\rho_0}{\partial r}\left[\sum\beta_l Y_{l0}-\frac{c}{4\pi}\sum\beta_l^2+\frac{1}{2}(r-R_0)R_0\times\left(\sum\beta_l\boldsymbol{\nabla}Y_{l0}\right)^2\right]+\frac{1}{2}R_0^2\frac{\partial^2\rho_0}{\partial r^2}\left(\sum\beta_l Y_{l0}\right)^2+\cdots, \tag{31}$$

where $\rho_0(r)$ has the usual Woods-Saxon form, β_i are the nuclear deformation parameters in Eq. (16) and $c=(R_0/2)(\int\rho_0 dr/\int\rho_0 r dr)$.

C. Simple estimate of the Schiff moment

Let us present a simple estimate of the nuclear Schiff moment in the case there is a T-, P-odd interaction and the nucleus possess a quadrupole and octupole deformation. One needs to calculate the *intrinsic* moment and the mixing coefficient α. We consider an axially symmetric nucleus which has a sharp surface and constant nucleon density ρ_t. The proton density can be approximated by constant $\rho = 3Z/4\pi R_0^3$. The intrinsic electric dipole moment in this approximation is zero, and only the first term in Eq. (5) contributes to the intrinsic SM. Using Eqs. (5), (16), and (17) and keeping only the terms containing β_2 and β_3 one gets, in accordance with Eq. (25),

$$S_{\rm intr} \equiv \frac{1}{10} e \int \rho r^2 z d^3\boldsymbol{r} = eZR_0^3 \frac{9}{20\pi\sqrt{35}} \beta_2\beta_3. \qquad (32)$$

Using then the deformation parameters $\beta_2 = 0.12$ and $\beta_3 = 0.1$, $R_0 = 1.2\times A^{1/3}$ fm, $A = 230$, and $Z = 88$ we obtain: $S_{\rm intr} = 10.4e$ fm^3.

The rotational states of an odd-mass nucleus can be written in terms of intrinsic states as

$$|IM\pm K\rangle = \left(\frac{2I+1}{8\pi^2}\right)^{1/2} D^I_{M\pm K}(\varphi,\vartheta,\psi)\varphi^{(A)}_{\pm K}(\boldsymbol{r}')\chi^{(A)}, \qquad (33)$$

where $D^I_{M\pm K}(\varphi,\vartheta,\psi)$ is a Wigner D function, $\chi^{(A)}$ is the wave function of the quadrupole and octupole deformed (reflection asymmetric) nuclear core in the intrinsic frame, and $\varphi^{(A)}_{\pm K}(\boldsymbol{r}')$ is the wave function of the unpaired nucleon in the intrinsic frame, with an angular momentum projection of $\pm K$ on the z' axis.

Let us now present an order of magnitude estimate of the mixing coefficient α which is needed to find the magnitude of the Schiff moment in the laboratory frame [see Eq. (15)]. $\hat{K} = \boldsymbol{In}$ and V^{PT} are both T-, P-odd pseudoscalars. Therefore, $\langle \varphi^{(A)}_{+K}|V^{PT}|\varphi^{(A)}_{+K}\rangle \propto K$ and so $\langle \varphi^{(A)}_{-K}|V^{PT}|\varphi^{(A)}_{-K}\rangle = -\langle \varphi^{(A)}_{+K}|V^{PT}|\varphi^{(A)}_{+K}\rangle$ (this fact can be easily supported by model calculations). Using this fact and Eqs. (33) and (9) we get $\langle \Psi^-|V^{PT}|\Psi^+\rangle = \langle \varphi^{(A)}_{+K}|V^{PT}|\varphi^{(A)}_{+K}\rangle$. If single-particle wave function $\varphi^{(A)}_{+K}$ was a good parity state this matrix element would be zero. However, due to the perturbation caused by the static octupole deformation of the nucleus (V_3), it is a combination of the opposite parity orbitals $\phi_{1,+K}$ and $\phi_{2,+K}$:

$$\varphi^{(A)}_{+K} = \phi_{1,+K} + \gamma\phi_{2,+K}, \qquad (34)$$

$$\gamma = \frac{\langle \phi_{2,+K}|V_3|\phi_{1,+K}\rangle}{E_1 - E_2}, \qquad (35)$$

$$\phi_{1,+K} = \mathcal{R}_1(r')\Omega_{j,l,+K}(\vartheta',\varphi'),$$

$$\phi_{2,+K} = \mathcal{R}_2(r')\Omega_{j,\tilde{l},+K}(\vartheta',\varphi') = -\mathcal{R}_2(r')(\boldsymbol{\sigma}\hat{\boldsymbol{r}}')\Omega_{j,l,+K}(\vartheta',\varphi'), \qquad (36)$$

where $\hat{\boldsymbol{r}} = \boldsymbol{r}/r$ is a unit vector along $\mathbf{r}$, Ω_{jlK} is a spherical spinor, $\tilde{l} = 2j - l$, e.g., $p_{3/2}$ and $d_{3/2}$ orbitals. (Of course there will also be an admixture of other states having different values of l,j. We neglect these states for simplicity.) The mixing coefficient γ is proportional to the parameter of the octupole deformation β_3. To make an estimate we assume that the single-particle potential $U(\boldsymbol{r})$ has the same form as the nuclear density $\rho_t(\boldsymbol{r})$. Using the expansion in Eq. (31) where $\rho_0(r') = \theta(R_0 - r')/(\frac{4}{3}\pi r_0{}^3)$ (where θ is the step function) we get

$$V_3 \approx U(0)R_0\beta_3\delta(R_0 - r')Y_{30}. \qquad (37)$$

Using Eq. (35) we then have

$$|\gamma| \simeq \left|\frac{\beta_3 U(0)\mathcal{R}_1(R_0)\mathcal{R}_2(R_0)R_0{}^3}{E_1 - E_2}\int \Omega_2^* Y_{30}\Omega_1 d\Omega'\right| \simeq \beta_3, \qquad (38)$$

where we have used $\mathcal{R}_1(R_0)\mathcal{R}_2(R_0) \approx 1.4/R_0{}^3$ [26], $|U(0)| \approx 50$ MeV, $|E_1 - E_2| \approx 5$ MeV, and $|\int \Omega_2^* Y_{30}\Omega_1 d\Omega'| \simeq 0.07$. Therefore, we have

$$\alpha = \frac{\langle \varphi^{(A)}_{+K}|V^{PT}|\varphi^{(A)}_{+K}\rangle}{E^+ - E^-} \simeq 2\beta_3 \frac{\langle \phi_{1,+K}|V^{PT}|\phi_{2,+K}\rangle}{E^+ - E^-}. \qquad (39)$$

Finally, we must estimate the matrix element between spherical orbitals $\langle \phi_{1,+K}|V^{PT}|\phi_{2,+K}\rangle$. Using Eq. (30) for the form of V^{PT} we get

$$V^{PT} = -\eta \frac{3G}{8\pi\sqrt{2}mr_0{}^3}(\boldsymbol{\sigma}\hat{\boldsymbol{r}}')\delta(R_0 - r'). \qquad (40)$$

Here $r_0 = 1.2$ fm is the internucleon distance. Using Eq. (36) and $(\boldsymbol{\sigma}\hat{\boldsymbol{r}}')^2 = 1$ gives

$$\langle \phi_{1,+K}|V^{PT}|\phi_{2,+K}\rangle = \eta \frac{3G}{8\pi\sqrt{2}mr_0{}^3}\mathcal{R}_1(R_0)\mathcal{R}_2(R_0)R_0{}^2 \approx \frac{\eta}{A^{1/3}} 1 \text{ eV}. \qquad (41)$$

Using $|E^+ - E^-| = 50$ keV, $\beta_3 = 0.1$ (see data in the tables), and Eqs. (39) and (41) gives (for $A = 230$) $|\alpha| \sim 2\beta_3 A^{-1/3}\eta$ eV$/|E^+ - E^-| \sim 7\times 10^{-7}\eta$. This provides the following estimate for the collective Schiff moment in the laboratory frame:

$$S \sim \alpha S_{\rm intr} \sim 0.05e\beta_2\beta_3{}^2 ZA^{2/3}\eta(r_0)^3 \text{ eV}/|E^+ - E^-| \sim 700\times 10^{-8}\eta e \text{ fm}^3. \qquad (42)$$

We see that the collective Schiff moment is about 500 times larger than the Schiff moment due to the unpaired nucleon in spherical nucleus, $S \simeq 1.5\times 10^{-8}\eta e$ fm^3 [18,35]. Note, however, the strong dependence of the collective Schiff moment on the deformation parameters.

We should remark here that this is a schematic calculation and more detailed and realistic calculations are presented in Secs. IV A, IV D, and V. Nevertheless the present estimate represents the essence of this theory and the order of magnitude estimate agrees with the detailed calculations.

D. Particle-core model for a reflection-asymmetric nucleus and *P*-, *T*-odd mixing of parity doublets

Any nucleus, whether even or odd mass, that is reflection asymmetric may possess *intrinsic* T-, P-odd moments. Such moments will exist in the *laboratory* frame only if there is also a T-, P-odd mixing between g.s. parity doublet levels. If the even-even nucleus is axially symmetric, a pseudoscalar T-, P-odd operator cannot mix $K=0$ doublet states which have identical intrinsic structure [38]. Besides, the energy splitting within parity doublets is systematically much less in odd (or odd-odd) than in neighboring even-even nuclei [39,14,40]. So in odd (or odd-odd) nuclei the mixing should be considerably larger. For this reason we consider odd nuclei in what follows.

We use here the particle-core model for a reflection-asymmetric nucleus [14,40]. The T-, P-odd as well as P-odd T-even mixing was studied in this model recently [41,38]. This model involves two $K^\pi=0^+$ and $K^\pi=0^-$ members of a parity doublet of the even-even core with the energy splitting E_c between them. The wave functions of these states χ^π are projections of the reflection-asymmetric core state χ_A [14]

$$\chi^\pi=\frac{1}{\sqrt{2}}(1+\pi\hat{P})\chi_A, \tag{43}$$

where $\hat{P}$ is the core parity operator. The single-particle states φ_A are solutions of the reflection-asymmetric single-particle plus pairing Hamiltonian $H_{\rm sp}+H_{\rm pair}$ (different forms of potentials such as folded Yukawa, deformed Woods-Saxon or Nilsson are used in $H_{\rm sp}$ [14,31,42,38]). The wave functions in the model are [14,38]

$$\Psi^{Ip}_{MK}=\left[\frac{2I+1}{16\pi^2}\right]^{1/2}[1+\hat{R}_2(\pi)]D^I_{MK}\Phi^p_K, \tag{44}$$

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 particle states ϕ^π we write (in the matrix notation $a\phi=\sum_k a_k\phi_k$)

$$\begin{aligned}\Phi^+&=a_+\chi^+\phi^++b_+\chi^-\phi^-,\\ \Phi^-&=a_-\chi^-\phi^++b_-\chi^+\phi^-.\end{aligned} \tag{45}$$

The matrix elements of V^{PT} are given by [38]

$$\begin{aligned}\langle\Psi^{I+}_{MK}|V^{PT}|\Psi^{I-}_{MK}\rangle=&\,a_+b_-\langle\phi^+_K|V^{PT}|\phi^-_K\rangle\\ &+a_-b_+\langle\phi^+_K|V^{PT}|\phi^-_K\rangle.\end{aligned} \tag{46}$$

(As already mentioned the pseudoscalar operator V^{PT} cannot connect doublet states of an even-even core χ^π because of the opposite rotational symmetry of these states [38] $\hat{R}_2\chi^\pi=\pi\chi^\pi$.)

The expectation value of a T-, P-odd operator $\hat{O}$ in a T-, P-admixed state $\tilde{\Phi}^+_i$ is

$$\langle\tilde{\Phi}^+_i|\hat{O}|\tilde{\Phi}^+_i\rangle=2\alpha_{ii}\langle\Phi^+_i|\hat{O}|\Phi^-_i\rangle+2\sum_{j\neq i}\alpha_{ij}\langle\Phi^+_i|\hat{O}|\Phi^-_j\rangle. \tag{47}$$

The matrix elements between core states are

$$\langle\chi^+|\hat{O}|\chi^-\rangle=\langle\chi_A|\hat{O}|\chi_A\rangle. \tag{48}$$

One can write the one-body operator $\hat{O}$ as the sum of core and particle terms $\hat{O}=\hat{O}_{\rm core}+\hat{O}_p$ and obtain

$$\begin{aligned}\langle\Phi^+_i|\hat{O}|\Phi^-_j\rangle=&\,\langle\chi_A|\hat{O}_{\rm core}|\chi_A\rangle(a_{+i}a_{-j}+b_{+i}b_{-j})\\ &+\langle\phi^+_i|\hat{O}_p|\phi^-_j\rangle a_{+i}b_{-j}\\ &+\langle\phi^+_j|\hat{O}_p|\phi^-_i\rangle a_{-j}b_{+i}.\end{aligned} \tag{49}$$

For $i=j$ this is just the intrinsic moment in the reflection-asymmetric core-particle state $\Phi=\chi_A\varphi_A\equiv\chi_A(a\phi^++b\phi^-)$. For closely spaced doublets $a_{+i}\approx a_{-i}$, $b_{+i}\approx b_{-i}$ and $(a_{+i}a_{-j}+b_{+i}b_{-j})\approx\delta_{ij}$. With respect to the single-particle contribution to a T-, P-odd moment in Eqs. (47) and (49) note that the admixture of the doublet level is considerably larger than the admixtures of the other levels of opposite parity, i.e., $\alpha_{ii}\gg\alpha_{ij}, i\neq j$. Neglecting these ''off-diagonal'' α_{ij} contributions one gets

$$\langle\tilde{\Phi}^+_i|\hat{O}|\tilde{\Phi}^+_i\rangle\approx2\alpha_{ii}(\langle\chi_A|\hat{O}_{\rm core}|\chi_A\rangle+\langle\varphi_A|\hat{O}_p|\varphi_A\rangle) \tag{50a}$$

and

$$\begin{aligned}\langle\tilde{\Psi}^{I+}_{MK}|\hat{O}_{\mu=0}|\tilde{\Psi}^{I+}_{MK}\rangle=&\,\langle IMl0|IM\rangle\langle IKl0|IK\rangle\\ &\times\langle\tilde{\Phi}^+_i|\hat{O}_{\mu=0}|\tilde{\Phi}^+_i\rangle,\end{aligned} \tag{50b}$$

where l is the rank of the operator. For a vector operator such as $\hat{\boldsymbol{S}}$ (or $\hat{\boldsymbol{d}}$) one obtains, in accordance with Eqs. (10), (14), and (15),

$$\langle\tilde{\Psi}^{I+}_{MK}|\hat{S}_z|\tilde{\Psi}^{I+}_{MK}\rangle=\frac{MK}{I(I+1)}2\alpha_{ii}(\langle\chi_A|\hat{S}_{\rm core}|\chi_A\rangle+\langle\varphi_A|\hat{S}_p|\varphi_A\rangle). \tag{51}$$

The intrinsic SM of the even Z core $\langle\chi_A|\hat{S}_{\rm core}|\chi_A\rangle$ is given by Eq. (27).

We stress again that the essential difference between the reflection-asymmetric (octupole deformed) nucleus and the reflection symmetric (quadrupole deformed) one is that the former has *intrinsic* T-, P-odd moments which are essentially *collective* since they involve contributions of the core nucleons. Note that in a nucleus which has a quadrupole deformation but no octupole deformation the ground state and its parity ''partner'' are built from a single good parity core state, e.g., χ^+, and therefore the coefficients in Eq. (45) are then $a_+=1$, $b_+=0$, $a_-=0$, $b_-=1$. So apart from a small core polarization contribution [18,35] there is no contribution from the core.

The parity mixing of a reflection asymmetric single-particle state $\varphi_A = \Sigma_k a_k \phi_k^+ + \Sigma_m b_m \phi_m^-$ is conveniently expressed via the expectation value of the single-particle parity operator $\hat{\pi}_p$ [14]:

$$\pi_p \equiv \langle \varphi_A | \hat{\pi}_p | \varphi_A \rangle = \sum_k a_k^2 - \sum_m b_m^2 . \tag{52}$$

Using this quantity one can write the admixture coefficient α_{ii} as

$$|\alpha_{ii}| \approx \left| \frac{\langle \phi_i^+ | V^{PT} | \phi_i^- \rangle}{E_i^+ - E_i^-} \right| \sqrt{(1-\pi_{pi}^2)}. \tag{53}$$

Here E_i^+ and E_i^- are the energies of the particle-core states Φ_i^+, Φ_i^-. The α_{ii} obviously is maximal for a doublet built on the strongly parity admixed ($|\pi_p| \ll 1$) intrinsic state. Note, that although the form of Eq. (53) is analogous (for $\pi_{pi}=0$) to the case when there is a close single-particle level of opposite parity in reflection-symmetric deformed nuclei [18], there is an important difference. Namely [18], if one neglects the spin-orbit interaction and assumes that the nuclear density $\rho_t(\boldsymbol{r})$ and the single-particle potential $U(\boldsymbol{r})$ have the same form then

$$V^{PT} \sim \boldsymbol{\sigma} \boldsymbol{\nabla} U(\boldsymbol{r}) = i[\boldsymbol{\sigma p}, H_{\rm sp}], \tag{54}$$

and the one-body matrix element $\langle \phi^+ | V^{PT} | \phi^- \rangle$is proportional to the energy difference

$$\langle \phi^+ | V^{PT} | \phi^- \rangle \sim i \langle \phi^+ | [\boldsymbol{\sigma p}, H_{\rm sp}] | \phi^- \rangle \sim e_{\phi^-} - e_{\phi^+}, \tag{55}$$

where e_{ϕ^+} and e_{ϕ^-} are the single-particle energies. In the case of a reflection symmetric (e.g., quadrupole deformed) nucleus $E^+ = e_{\phi^+}$ and $E^- = e_{\phi^-}$. The mixing coefficient is therefore enhanced only in a few cases when single-particle deformed levels are accidentally close and the approximation of Eqs. (54) and (55) becomes a crude one [18]. In the reflection-asymmetric case always [14,40,38]

$$|E^+ - E^-| \lesssim \frac{E_c |e_{\phi^+} - e_{\phi^-}|}{2|\langle \phi^+ | V_{\rm odd} | \phi^- \rangle|} \ll |e_{\phi^+} - e_{\phi^-}|, \tag{56}$$

where $V_{\rm odd}$ is the reflection-asymmetric part of the single-particle Hamiltonian $H_{\rm sp}$. Therefore the admixture coefficient α_{ii} is generally enhanced relatively to that in spherical or quadrupole deformed nuclei. The splitting within the parity doublet (for $K \neq \frac{1}{2}$) can be also written as [14,40]

$$|E^+ - E^-| \simeq |E_c \pi_p|, \tag{57}$$

exhibiting the reduction of splitting for an odd nucleus in comparison with the splitting of parity doublet states of the even-even core. In the case of $K=\frac{1}{2}$ doublets the Coriolis interaction, leading to an additional splitting within doublets is included in the model [38].

Let us look now at the single-particle part of the SM given by Eqs. (5), (49), and (50). The ''diagonal'' single-particle contribution in Eq. (50a) can be written as

$$2\alpha_{ii} \langle \phi_i^+ | \hat{O}_p | \phi_i^- \rangle (a_{+i} b_{-i} + a_{-i} b_{+i}) \approx 2 \langle \phi_i^+ | \hat{O}_p | \phi_i^- \rangle \frac{\langle \phi_i^+ | V^{PT} | \phi_i^- \rangle}{E_i^+ - E_i^-} (1-\pi_{pi}^2). \tag{58}$$

Thus, in general, due to the enhancement in α_{ii} the single-particle contribution of the odd proton is enhanced relatively to the case of a quadrupole deformed but reflection symmetric nucleus. In the proton-odd nuclei the single proton contributes to both terms of the SM operator in Eq. (5). These terms are of the same order and partially cancel. In the neutron-odd nuclei the single neutron contribution to the SM operator in Eq. (5) enters only through the corrections to the dipole moment term and therefore is very small.

As is shown in Ref. [14] the effects of BCS-like pairing are maximal when the Fermi level is exactly halfway between the single-particle levels. In this case the simplest model of two opposite parity single-particle levels results in an exactly degenerate parity doublet. In realistic calculations the effect of pairing correlations on single-particle levels is revealed only in somewhat altered energy splittings between members of parity doublets. In the calculations of matrix elements of parity and parity and time reversal violating potentials and single-particle parts of electric moments, the effect of pairing is more important. When one uses the BCS quasiparticle states instead of single-particle states, the matrix elements of the operators V^{PT}, V^{PV} and $\hat{O}_p$ are to be multiplied by pairing factors $u_f u_i + c_{\rm sym} v_f v_i$, where $c_{\rm sym}$ depends on the symmetry properties of the operator under the time reversal and Hermitian conjugation [24,26]. For Hermitian operators, $c_{\rm sym}=1$ if an operator is T odd and $c_{\rm sym}=-1$ if it is T even [26]. Thus, for the T-odd V^{PT}, one has the factor $u_f u_i + v_f v_i$, whereas for the T-even V^{PV} and a single-particle matrix element of an electric operator $\hat{O}_p$ the corresponding factor is $u_f u_i - v_f v_i$. The difference in signs in the expressions for pairing correlation factors is related to the fact that matrix element of V^{PV} operator between members of a parity doublet goes to zero when the doublet becomes degenerate while the matrix element of V^{PT} operator does not vanish [43,38,44].

V. CALCULATIONS AND ESTIMATES

A. Nuclear structure calculations

The set of deformation parameters β_l (up to $l=6$) was taken from Ref. [13] where it was calculated using a deformed Woods-Saxon single-particle potential and Strutinsky shell correction method. From the sets of deformations, calculated in Ref. [13], we have chosen those which correspond to the experimental value of K in the g.s. This set is shown in Table I. The particle-core wave functions were calculated using the reflection-asymmetric particle core model [14]. In an attempt to be consistent we calculated both the intrinsic T-, P-odd moments and admixture coefficients using basically the same single-particle potential and shell correction parameters. The computer code WSBETA [42] and the ''universal'' set of parameters was used in calculations involving deformed single-particle Woods-Saxon potential. (A modification of the code was made to include explicitly the β_1 deformation.)

TABLE I. Intrinsic g.s. deformations and energy splittings between opposite parity core states.

	^{223}Ra	^{225}Ra	^{223}Rn	^{221}Fr	^{223}Fr	^{225}Ac	^{229}Pa
β_2	0.125	0.143	0.129	0.106	0.122	0.138	0.176
β_3	0.100	0.099	0.081	0.100	0.090	0.104	0.082
β_4	0.076	0.082	0.078	0.069	0.076	0.078	0.093
β_5	0.042	0.035	0.024	0.045	0.033	0.038	0.020
β_6	0.018	0.016	0.023	0.020	0.022	0.013	0.015
E_c (keV)	212	221	213	305	212	206	333

To check the stability of the values of admixture coefficients we calculated them also using a Nilsson potential with ϵ_l deformations approximately corresponding to the same nuclear surface (see, e.g., Ref. [45]). It is known [46] that there are some differences in the energies and wave functions when calculated with deformed Nilsson or Woods-Saxon potentials in the actinide region. Especially the proton levels are different because of the fact that the Coulomb term is included in the Woods-Saxon potential but is only simulated in the Nilsson potential. Because of that we performed calculation of α admixtures with the Nilsson potential only for the neutron-odd nuclei. For the Nilsson potential we used parameters of Ref. [46] which are known to produce a good fit to experimental data. See for example the reflection-asymmetric calculations of ^{225}Ra in Ref. [47].

The energy splittings of the core parity doublets, E_c, and moments of inertia were taken from Ref. [31]. The values of E_c we used are given in Table I. The effect of the $l=1$ deformation (β_1 or ϵ_1) in the deformed single-particle potential on the energies and admixture coefficients of doublets is small. However this deformation is important for the calculation of the shell correction to the intrinsic Schiff moment.

For the BCS treatment of pairing we used the strength parameter $G_{p,n}$ [48]

$$G_{p,n}=\frac{1}{A}\left(g_0 \pm g_1 \frac{N-Z}{A}\right), \tag{59}$$

with $g_0=19.2$ MeV, $g_1=7.4$ MeV for neutrons and $g_0=22.0$ MeV, $g_1=8.0$ MeV for protons. We found that the admixture coefficients, as well as other properties of these nuclei calculated in Ref. [31], are not sensitive to the pairing strength (or gap parameter Δ). The standard Strutinsky shell correction calculation of the smoothed single-particle occupation numbers n was performed using parameters taken from Ref. [34].

The intrinsic SM was calculated using Eqs. (27) and (28). The ''macroscopic'' term $S^M_{\rm intr}$ was computed directly using Eqs. (5) and (19) with $C=27$ MeV which is the droplet model value [29]. We calculated the shell correction for the first term of the intrinsic SM operator in Eq. (5). This correction strongly depends on the proton number and for $86 \leqslant Z \leqslant 91$ its absolute value decreases with increasing of Z. For $Z<92$ it has a negative sign relatively to $S^M_{\rm intr}$ and changes from 33% for $^{223}_{86}$Rn to 9% for $^{225}_{89}$Ac. In case of proton-odd nuclei we calculated also the single proton contribution to the SM. For the g.s. of ^{223}Fr, ^{225}Ac, and ^{229}Pa it amounts to 2–5 % of the corresponding values of $S^M_{\rm intr}$. The resulting intrinsic Schiff moments of octupole deformed nuclei are in the range (15–28)e fm^3. We estimate that when we allow for reasonable changes in the parameters used, and when other corrections (not treated here) are introduced the *intrinsic* SM will change by 30% at most. Thus we believe, that the uncertainties in the evaluated values of the *intrinsic* SM are of the same order.

The computed values of *intrinsic* Schiff moments, admixture coefficients, and resulting Schiff moments in the laboratory system as well as the calculated and experimental energy splitting for the g.s. parity doublets and calculated parities π_p of the intrinsic single-particle g.s. are all given in Table II.

The main uncertainty in the entire calculation of Schiff moments in the laboratory frame arises from the estimate of admixture coefficients α, which are calculated using theoretical values of the energy splitting between members of the doublets. In our calculations the first state above the Fermi level which has the same value of K as the experimentally determined g.s. was chosen to be the g.s. level. In the work of Leander and Chen [31] the nonadiabatic Coriolis coupling and other refinements were introduced (in some cases also adjustments of quasiparticle energies were made), which allowed to describe properties of g.s. and excited levels. We

TABLE II. Admixture coefficients α (absolute values) and theoretical energy splitting between the g.s. doublet levels $\Delta E=E^- - E^+$, parities of the intrinsic (reflection-asymmetric) single-particle g.s. calculated using the Woods-Saxon (WS) and Nilsson (Nl) potentials, experimental energy splitting, *intrinsic* Schiff moments and Schiff moments calculated with the Woods-Saxon potential, and induced atomic dipole moments. The values for ^{199}Hg, ^{129}Xe, and ^{133}Cs from Refs. [35,57,18] are given for comparison.

	^{223}Ra	^{225}Ra	^{223}Rn	^{221}Fr	^{223}Fr	^{225}Ac	^{229}Pa	^{199}Hg	^{129}Xe	^{133}Cs
$\alpha(WS)(10^7\eta)$	1	2	4	0.7	2	3	34			
$\Delta E(WS)$ (keV)	170	47	37	216	75	49	5			
π_p(WS)	0.81	-0.02	0.17	-0.55	-0.34	-0.35	0.01			
$\alpha(Nl)(10^7\eta)$	2	5	2							
$\Delta E(Nl)$ (keV)	171	55	137							
$\Delta E_{\rm expt}$ (keV)	50.2	55.2		234	160.5	40.1	0.22			
$S_{\rm intr}(e$ fm$^3)$	24	24	15	21	20	28	25			
$S(10^8\eta e$ fm$^3)$	400	300	1000	43	500	900	1.2×10^4	-1.4	1.75	3
d(at) $(10^{25}\eta e$ cm)	2700	2100	2000	240	2800			5.6	0.47	2.2

did not include couplings between states with different K and did not adjust model parameters to fit properties of individual states. In some cases the states calculated as the lowest ones above the Fermi surface do not have the experimentally determined values of K [13]. For example, the $I=\frac{7}{2}$ g.s. of ^{223}Rn which was described in [31] as arising from Coriolis coupling of $K=\frac{7}{2}$ and $K=\frac{1}{2}$ states, is not the lowest state in our calculation but is 270 keV above the g.s. Thus it cannot be ruled out that in some cases some single-particle states close to the Fermi level and different from the ones we chose, fit better the g.s. parity doublet. The absolute values of the admixture coefficients for the doublet which was taken as the g.s. are for all nuclei we calculated (except ^{229}Pa which has an exceptionally small energy splitting in the g.s. parity doublet) in the range $(1–5)\times 10^{-7}\eta$ for both reflection asymmetric Woods-Saxon and Nilsson single-particle potentials. If we consider also admixture coefficients for the two parity doublets closest to the g.s. parity doublet which have the same K the range is $(0.15–5)\times 10^{-7}\eta$. We remark that because the one-body P-, T-odd potential V^{PT} in Eq. (30) is proportional to the derivative of the density of nucleons and thus is surface-peaked, its matrix elements depend on the behavior of the single particle wave functions in the nuclear surface region and hence may vary significantly from level to level.

The values of the Schiff moments in the laboratory system *and the resulting atomic dipole moments given in Table II are computed using the Woods-Saxon single-particle potential, whereas in Ref. [8] they were evaluated using the Nilsson potential.* The admixtures α calculated here with the Nilsson potential are only slightly different (due to pairing correction) from those in Ref. [8]. As already noted the main source of difference in the values of S and $d(\mathrm{at})$ given in Table II and in Ref. [8] is the variation of admixture coefficients α for the two potentials.

As one sees in Table II some of parities π_p depart considerably from ± 1 meaning that these orbitals are strongly parity mixed, which is one of the reasons for large admixture coefficients α. Equation (57) describes well the splittings within the doublets except for the $K=\frac{1}{2}$ cases of the ^{225}Ra and ^{221}Fr g.s., where there is an additional Coriolis splitting [14,38]. For ^{225}Ra, ^{221}Fr, and ^{225}Ac the experimental energy splitting between members of the g.s. parity doublet is well reproduced in our calculation whereas in ^{223}Fr and ^{223}Ra nuclei it differs by a factor of 2 or 3. For ^{223}Rn no data on doublets are available. We should remark here that in view of Eq. (55) one can expect some correlation between the matrix element of V^{PT} and the energy splitting within the doublet. We expect therefore that the use of experimental energy splittings will not necessarily lead to more precise values for the admixture coefficients α.

The nuclear Schiff moments for the octupole deformed nuclei calculated here are about two orders of magnitude larger that those obtained in Refs. [18,35] for isotopes of ^{129,131}Xe, ^{199,201}Hg, and ^{203,205}Tl. As already mentioned the enhancements we discuss are for nuclei with asymmetric shapes and therefore there is also two orders of magnitude enhancement with respect to nuclei such as ^{161}Dy and ^{237}Np [18] which have large quadrupole deformation. These nuclei have close to the g.s. levels of the same spin and opposite parity as the g.s., but are believed to be reflection symmetric.

The SM's in even Z nuclei such as Xe and Hg are caused mainly by the polarization of protons in the core by the T-, P-odd field of the external nucleon [see Eq. (29)]. Therefore, the SM is proportional to the η_{np} constant. It was demonstrated in [35] that this ''polarization'' mechanism gives SM of the same order of magnitude as in nuclei that have a proton outside the core. Many-body corrections give also contributions proportional to other T-, P-odd constants, e.g., η_{nn}. In our calculations the interaction of the odd proton or neutron with the even-even core and the nuclear SM in the laboratory system are expressed via the effective constant η.

The experimental data regarding the nuclei we consider are discussed in the reviews [31,10–12]. The ^{223}Ra and ^{225}Ra nuclei were also considered in detail in Refs. [49,47]. In both ^{221,223}Rn isotopes the $I=\frac{7}{2}$ g.s. spin was determined using laser spectroscopy methods [50], and no data on excited levels are presently available. The computed deformations in these two isotopes calculated in Ref. [13] are similar. Using the Coriolis coupling Leander and Chen [31] were able to reproduce spectroscopic characteristics of g.s. somewhat better for ^{223}Rn than for ^{221}Rn. We made a calculation for ^{223}Rn because its $I=\frac{7}{2}$ g.s. is easier to interpret theoretically [13,31].

The case of Fr is especially interesting in light of the recent experiments involving trapping of Fr atoms [51]. The latest experimental and theoretical studies of ^{221}Fr [52] and ^{223}Fr [53,54] provide strong evidence of intrinsic reflection asymmetry in the g.s. The g.s of ^{221}Fr is $K^{\pi}=\frac{1}{2}^{-}$, $I^{\pi}=\frac{5}{2}^{-}$. The assignment of the doublet $K^{\pi}=\frac{1}{2}^{+}$, $I^{\pi}=\frac{5}{2}^{+}$ state at 234 keV was suggested in [52]. The result for the Schiff moment of ^{221}Fr is smaller than that of ^{223}Fr because of the following factors. Firstly, the factor $MK/I(I+1)$ in Eq. (51) is $\frac{1}{7}$ for ^{221}Fr, whereas for $I=\frac{3}{2}$, $K=\frac{3}{2}$ g.s. of ^{223}Fr it is $\frac{3}{5}$. Secondly our calculation gives the admixture coefficient α for ^{221}Fr about 3 times less than for ^{223}Fr. Because of these factors the Schiff moment of ^{221}Fr in the *laboratory* frame is about 12 times less than that of ^{223}Fr, although in the *intrinsic* frame the values of S_{intr} are roughly equal.

There is a controversy regarding the g.s. spin and parity doublet in ^{229}Pa, which is on the border of the region of octupole deformed nuclei. Two assignments: (a) $K=\frac{5}{2}$, $I=\frac{5}{2}$ g.s. and 220 eV energy splitting within the parity doublet [11,55] and (b) $K=\frac{1}{2}$, $I=\frac{3}{2}^{-}$ g.s. and unidentified parity partner level [56,12] were made. In case (a) our calculations give using the experimental value of the energy splitting the admixture coefficient $\alpha=640\times 10^{-7}\eta$ and the Schiff moment in the laboratory frame, $S=230\,000\times 10^{-8}\eta e$ cm. Note however that in Table II the results for ^{229}Pa are an order of magnitude smaller because a theoretical value of 5 keV was used for the energy splitting of the doublet.

B. Calculation of atomic electric dipole moments

Atomic electric dipole moment can be calculated using Eq. (7). However, we do not need new complicated numerical calculations to find the EDM of interest. We can use numerous calculations for the lighter atomic analogs (Xe, Hg, Cs) and introduce corresponding corrections taking into account the Z dependence of the effect to find EDM of heavy atoms (Rn, Ra, and Fr correspondingly). Indeed, it follows from the atomic calculations that atomic EDM in Eq. (7) is saturated by the contributions of electrons from the external shells which are similar in the analogous atoms (the energy denominators for the transitions from these shells are small and radial integrals are large). The expression for the atomic EDM is a product of three factors: matrix elements of the radius $\langle k_1|r_z|k_2\rangle$, energy denominators $E_{k_1}-E_{k_2}$ and matrix elements of the T-, P-odd nuclear electric potential $\langle k_1|-e\varphi^{(3)}|k_2\rangle$. The first two factors are determined by the wave functions at large distances and they are the same in analogous atoms. This fact is deduced from numerous semiempirical and computer calculations, from experimental data for energy levels and probabilities of electromagnetic transitions, as well as from the data on atomic polarizabilities for analogous atoms (the expression for the polarizability also contains radial integrals and energy denominators). The matrix elements $\langle k_1|-e\varphi^{(3)}|k_2\rangle$ are determined by the wave function at small distances (more accurately, by the gradient of the external electron density at the nucleus) which strongly depends on the nuclear charge. However, this dependence was calculated analytically [18]. The contribution of the Schiff moment is determined by the matrix element between $s_{1/2}$ and $p_{1/2}$ (or $s_{1/2}$ and $p_{3/2}$) electron orbitals which is proportional to $SZ^2R_{1/2}$ (or $SZ^2R_{3/2}$). The number of $p_{3/2}$ states is two times larger than the number of $p_{1/2}$, therefore we will need linear combination of the relativistic factors $R_{sp}=(R_{1/2}+2R_{3/2})/3$.

The relativistic factors $R_{1/2}$ and $R_{3/2}$ are given by

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

$$R_{3/2}=\frac{48}{\Gamma(2\gamma_{1/2}+1)\Gamma(2\gamma_{3/2}+1)}\left(\frac{2ZR_0}{a_B}\right)^{\gamma_{1/2}+\gamma_{3/2}-3}, \tag{60}$$

where $\gamma_j=[(j+\frac{1}{2})^2-(Z\alpha)^2]^{1/2}$, a_B is the Bohr radius and R_0 is the nuclear radius. In light atoms $R_{sp}\simeq 1$, in heavy atoms $R_{sp}\simeq 10$. Thus, we have simple estimates of the electric dipole moments of Ra, Rn, and Fr induced by the nuclear Schiff moments:

$$d_{\mathrm{at}}(\mathrm{Ra})=d_{\mathrm{at}}(\mathrm{Hg})\frac{(SZ^2R_{\mathrm{sp}})_{\mathrm{Ra}}}{(SZ^2R_{\mathrm{sp}})_{\mathrm{Hg}}},$$

$$d_{\mathrm{at}}(\mathrm{Rn})=d_{\mathrm{at}}(\mathrm{Xe})\frac{(SZ^2R_{\mathrm{sp}})_{\mathrm{Rn}}}{(SZ^2R_{\mathrm{sp}})_{\mathrm{Xe}}},$$

$$d_{\mathrm{at}}(\mathrm{Fr})=d_{\mathrm{at}}(\mathrm{Cs})\frac{(SZ^2R_{\mathrm{sp}})_{\mathrm{Fr}}}{(SZ^2R_{\mathrm{sp}})_{\mathrm{Cs}}}, \tag{61}$$

where only the nuclear Schiff moment contributions to atomic EDM's d_{at} of Hg, Xe, and Cs are taken into account. The atomic structure ratios here are

$$\frac{(Z^2R_{\mathrm{sp}})_{\mathrm{Ra}}}{(Z^2R_{\mathrm{sp}})_{\mathrm{Hg}}}=1.6,$$

$$\frac{(Z^2R_{\mathrm{sp}})_{\mathrm{Fr}}}{(Z^2R_{\mathrm{sp}})_{\mathrm{Cs}}}\simeq\frac{(Z^2R_{\mathrm{sp}})_{\mathrm{Rn}}}{(Z^2R_{\mathrm{sp}})_{\mathrm{Xe}}}=7.7. \tag{62}$$

The calculation of EDM of Hg, Xe, and Cs has been done in Refs. [18,57,35]. The results of our calculations for Ra, Rn, and Fr are presented in Table II.

VI. SUMMARY

In this paper we studied the T-odd, P-odd electric moments in heavy nuclei with intrinsic reflection asymmetry and induced electric dipole moments in corresponding atoms. We presented a detailed theory of the collective T-, P-odd electric moments in reflection asymmetric odd-mass nuclei, in particular the Schiff moment. We employed the two-fluid liquid drop model, particle plus core model, and used the results of Nilsson-Strutinsky mean field calculations for intrinsic reflection asymmetric nuclear shapes. Various corrections for nuclear T-odd, P-odd electric moments were evaluated.

In the calculations of induced atomic electric dipole moments we employed the scaling relations between such moments in heavy atoms and their lighter analogs and used the results of the calculations for the latter to find the corresponding moments in heavy atoms. We studied the cases of all the heavy reflection-asymmetric odd-mass nuclei for which there is evidence of intrinsic octupole deformation in the ground state and which are relatively long lived, so their atoms could be suitable for experiment.

The results can be summarized in the following form.

(a) In a reflection asymmetric nucleus which has odd mass number or is odd-odd, enhanced collective T-odd, P-odd electric moments appear, if T-odd, P-odd terms are present in the nuclear Hamiltonian.

(b) The T-odd, P-odd Schiff moments in heavy nuclei with intrinsic reflection asymmetry are typically enhanced by more than 2 orders of magnitude in comparison with reflection-symmetric deformed or spherical nuclei.

(c) Due to the atomic structure effects, atomic electric dipole moments in heavy atoms are enhanced, compared to the lighter analogs. For atoms of nuclei with Z around 90, the atomic enhancement is of about 8 times, in comparison with analog atoms with Z around 55. This enhancement factor is about 2 compared to analogs with Z around 80.

(d) The atomic electric dipole moments, induced by T-odd, P-odd hadron-hadron interaction in the nuclei studied are typically enhanced 400–1000 times in comparison with Hg and Xe nuclei, for which the best experimental upper limits on atomic electric dipole moments are obtained. These findings may open new experimental possibilities of studying time reversal violation.

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APPENDIX: SCREENED *T*-, *P*-ODD ELECTROSTATIC POTENTIAL OF A NUCLEUS AND THE SCHIFF THEOREM

The Hamiltonian of an atom placed in a homogeneous external electric field $\boldsymbol{E}_0$ is

$$H=\sum_i \left[K_i-e\varphi_0(\boldsymbol{R}_i)-e\boldsymbol{R}_i\boldsymbol{E}_0\right]+\sum_{i>k}\frac{e^2}{|\boldsymbol{R}_i-\boldsymbol{R}_k|}-\boldsymbol{d}\boldsymbol{E}_0,$$

$$\varphi_0(\boldsymbol{R}_i)=e\int\frac{\rho(\boldsymbol{r})d^3\boldsymbol{r}}{|\boldsymbol{R}_i-\boldsymbol{r}|}. \qquad \text{(A1)}$$

Here K_i and $\boldsymbol{R}_i$ are the kinetic energy and coordinate of the electron, $\varphi_0(\boldsymbol{R}_i)$ is the electrostatic nuclear potential and $\boldsymbol{d}$ is the nuclear dipole moment. We consider the case of an infinitely heavy nucleus. The nuclear recoil correction by itself is not enough to generate an atomic EDM. This can easily be seen for the limit of a pointlike nucleus [22,23]. The atomic EDM occurs due to the finite size of the nucleus [23] [see Eqs. (4)–(7)]. The recoil correction times the correction due to finite size is extremely small. Let us add to H an auxiliary term

$$V=\boldsymbol{d}\boldsymbol{E}_0-\frac{1}{eZ}\sum_i \boldsymbol{d}\boldsymbol{\nabla}_i\varphi_0(\boldsymbol{R}_i). \qquad \text{(A2)}$$

It is easy to demonstrate that in the linear approximation in $\boldsymbol{d}$ the interaction V does not produce any energy shift, $\langle V\rangle=0$. Indeed

$$\frac{i}{m}\left[\sum_i \boldsymbol{p}_i,H\right]=-e\sum_i \boldsymbol{\nabla}_i\varphi_0(\boldsymbol{R}_i)+Ze\boldsymbol{E}_0. \qquad \text{(A3)}$$

We have taken into account that the total electron momentum $\Sigma_i\boldsymbol{p}_i$ commutes with the electron-electron interaction term. Using Eq. (A2) and $\langle n|[H,\Sigma_i\boldsymbol{p}_i]|n\rangle\sim(E_n-E_n)=0$ we obtain $\langle V\rangle=\boldsymbol{d}\boldsymbol{E}_0-(1/eZ)eZ\boldsymbol{d}\boldsymbol{E}_0=0$.

To find an electric dipole moment one needs to measure a linear energy shift in an external electric field. Since V does not contribute to this shift we can add it to the Hamiltonian

$$\tilde{H}\equiv H+V=\sum_i \left[K_i-e\varphi(\boldsymbol{R}_i)-e\boldsymbol{R}_i\boldsymbol{E}_0\right]+\sum_{i>k}\frac{e^2}{|\boldsymbol{R}_i-\boldsymbol{R}_k|},$$

$$\varphi(\boldsymbol{R}_i)=\varphi_0(\boldsymbol{R}_i)+\frac{1}{eZ}\boldsymbol{d}\boldsymbol{\nabla}_i\varphi_0(\boldsymbol{R}_i). \qquad \text{(A4)}$$

Note, that the Hamiltonian $\tilde{H}$ does not contain the direct interaction $\boldsymbol{d}\boldsymbol{E}_0$ between the nuclear electric dipole moment and external field (Schiff theorem [22,23]). The dipole term is also canceled out in the multipole expansion of $\varphi(\boldsymbol{R}_i)$.

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