NUCLEAR STRUCTURE
AND THE SEARCH FOR COLLECTIVE ENHANCEMENT
OF $\mathcal{P}, \mathcal{T}$-VIOLATION

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I. INTRODUCTION

It became already a common understanding that enables one to claim that “the nucleus is a natural laboratory for studying violation of fundamental symmetries”. Indeed, the existence of a broad class of self-sustaining systems bound by strong interactions, with the possibility to apply electric and magnetic fields and to observe the processes governed by weak interactions, allows one to experimentally select and amplify the phenomena signaling such violations. The classical example is given by parity non-conservation discovered in the experiment by Wu et al. with the use of the polarized $^{60}$Co nucleus. Another typical feature that characterizes the same case is the pre-existence of theoretical ideas predicting possible parity non-conservation.

Parity non-conservation in nuclear beta-decay is a large effect, essentially on the maximum possible level (the coefficient of angular correlation between the beta-electron and nuclear spin is, as follows from the left-current interaction mechanism, $\alpha = -v/c$, close to one). Therefore it is currently used as a tool for extracting important information on aspects of nuclear structure unrelated to weak interactions. As an example, we can mention the developing idea of utilizing the interference of electromagnetic and weak interactions for a measurement of the neutron skin in heavy nuclei (the “weak charge” of the proton in the standard model is only 0.08 of the neutron weak charge). Such data, still unavailable, would be instrumental for information on nuclear symmetry energy and the equation of state of neutron matter.
In general, the main interest to violation of fundamental symmetries can be explained by
the search for the effects beyond the predictions of the standard model\[^6\]. Among other
problems, such violations can provide a key to the understanding of one of the critical scientific
puzzles, the baryon asymmetry of the universe. One of the famous Sakharov conditions
for baryogenesis of asymmetry\[^7\] is the $\mathcal{CP}$-violation, which is equivalent, according to the
$\mathcal{CPT}$-theorem, to the violation of the time-reversal ($T$) invariance. The small effects of
$\mathcal{CP}$-violation known from experiments with neutral $K$- and $B$-mesons\[^8\] set limits on the
deviations from the standard model. We still do not have numbers which would show the
strength of $\mathcal{CP}$-violation in nucleon-nucleon and/or quark-quark forces. Our best hopes in
this direction are connected with atomic and nuclear experiments\[^9\].

In contrast to the beta decay, here we are interested in the specific properties of minor
components of stationary atomic and nuclear states. The non-orthodox features can be
better seen in phenomena fully forbidden by standard physics. Since anyway these effects
are numerically small, the main idea is to use the atomic or/nuclear environment as a
possible amplifier of non-standard properties. The experience of last decades confirms that
this idea may work.

As a striking example we can remind the reader the strong enhancement of the parity vi-
olation in scattering of slow longitudinally polarized neutrons off heavy targets first measured
in Dubna\[^10\] and then studied in detail at Los Alamos, see review articles\[^11, 12, 13, 14\]
and references therein. The relative difference of cross sections for neutrons of right and
left longitudinal polarization can reach 10%, whereas simple estimates based on a typical
strength of weak interactions would give $10^{-(7-8)}$. The enhancement by six orders of magni-
tude comes from the combination of high density of $p$-wave and $s$-wave resonances, uniformly
chaotic wave functions of compound states, and the large kinematic ratio of neutron widths
$\Gamma_s/\Gamma_p$ for the resonances mixed by $\mathcal{P}$-violating forces. This enhancement was anticipated
long ago\[^15\], theoretically predicted before the measurements by Sushkov and Flambaum
\[^16, 17\] and discussed in detail in\[^18, 19\].

A related, and probably even less expected, enhancement by 3-4 orders of magnitude
was observed in the asymmetry of the fragments from nuclear fission by slow polarized
neutrons with respect to the neutron polarization, see the review of the first experiments
in\[^20\]. Here the explanation\[^17\] again is based on a chaotic character of intrinsic nuclear
dynamics\[^21, 22\]. The kinematic enhancement factor is absent but the new element is that,
after the weak interaction has mixed compound levels of opposite parity, the pear-shaped
nucleus with parity doublets (an analog of Λ-doubling in molecules [23]) proceeds through
few specific fission channels which preserve memory of parity non-conservation. The later
Grenoble experiments [24] confirmed this scenario showing that the mixing occurred in a
“hot” nucleus between chaotic wave functions, and therefore the resulting asymmetry is
practically independent on the mass and kinetic energy distributions determined at the next
stages of the process.

We mentioned above the impressive nuclear phenomena related to parity non-
conservation. The $T$-violation was searched in various nuclear reactions [25] but also in
nuclear structure, namely in chaotic regions of complex spectra of excited nuclear states
[26]. The character of level repulsion at small spacings critically depends on the presence
or absence of time-reversal invariance of the Hamiltonian: the probability of having two
levels of the same symmetry class at a small spacing $s$ behaves as $s$ and $s^2$ with and without
$T$-invariance, respectively. Because of poor statistics for closely spaced avoided level cross-
ings, in practice such analysis produces only a rough upper boundary. The most interesting
and promising direction is related to the experimental search for electromagnetic multipoles
forbidden by discrete symmetries. As explained in the next section, the measurement of a
non-vanishing expectation value $\langle d \rangle$ of the electric dipole moment (EDM) $d$ of the atom
would be a direct proof of the existence in atoms and nuclei of the interactions violating
simultaneously $P$- and $T$-symmetry [27, 28]. The search for the atomic EDM is going on in
few experimental groups; right now the best boundaries are established for $^{129}$Xe and $^{199}$Hg. Our short review is devoted to the discussion of nuclear dynamics which could
amplify the EDM and therefore facilitate those hard and time-consuming experiments.

The ideas of possible nuclear enhancement of the atomic effects are important for choosing
the right nuclear isotope with largest odds of the successful measurement. In contrast to
the statistical enhancement of parity non-conservation in neutron scattering, the EDM is
to be found in the ground state of the atom and the nucleus. Here one cannot hope to
profit from the uniformly chaotic states at high level density. The chances to get significant
enhancement are related either to the more or less accidental close proximity of levels capable
of being mixed by the weak interactions [31], or with possible collective effects which could
coherently enhance the atomic EDM. In the EDM problem, the desired effects might be
associated with the combination of the quadrupole and octupole collectivity, either in the
form of static deformation, or in the interplay of corresponding soft vibrational modes. These ideas will be discussed in detail below. Apart from the direct goal to find the source for the enhancement of weak interactions, such studies are interesting by itself, as a many-body problem going beyond standard mean-field and random phase approximations.

We start with the explanation, Sec. 2, of the role of the nuclear Schiff moment as a mediator of $\mathcal{P}, \mathcal{T}$-odd forces between the nucleus and atomic electrons. We also briefly go through the list of current experimental approaches to search for the EDM. A simple single-particle contribution to the Schiff moment is discussed in Sec. 3. Sec. 4 describes the enhancement that is possible in heavy nuclei under simultaneous presence of static quadrupole and octupole deformation. In Sec. 5 we proceed with the further ideas substituting the permanent deformation with the large-amplitude vibrations of corresponding multipolarities. The appropriate conditions may exist in radioactive isotopes of radium, radon and thorium. These ideas are more speculative since the fully realistic calculations were not performed yet. Sec. 6 contains a short summary.

II. EDM AND SCHIFF MOMENT

A. EDM and fundamental symmetries

The electric dipole moment of the static charge distribution in the atom is given by the expectation value of the operator $\hat{d} = \sum_a e_a r_a$ in the ground state of the atom, where the subscript $a = 1, ..., Z$ enumerates atomic electrons. The dipole operator is a polar, i.e. $\mathcal{P}$-odd, $\mathcal{T}$-even, vector. In order to have a non-zero expectation value of any vector, the stationary state must have non-zero angular momentum. We will denote the total atomic spin $J$ and the nuclear spin $I$. This excludes closed shell atoms and nuclei. Nuclear spin $I \neq 0$ requires an odd mass number. In fact, the nuclei of current experimental interest, such as $^{129}$Xe, $^{199}$Hg, and $^{225}$Ra, have $I = 1/2$ which might be advantageous since the time-reversed magnetic substates $M_I = \pm 1/2$ are not split by external electric fields.

The rotational invariance supposedly remains exact even in the presence of weak interactions. This implies the well known relations between the matrix elements of any vector and those of angular momentum. Inside the rotational multiplet of states $|J M\rangle$, the EDM acts
as an effective operator

\[ \hat{d} = \frac{\langle d \cdot J \rangle}{J(J+1)} \hat{J}; \]  

(1)

here and below we mark by a hat the quantities where it is important to stress the operator nature. If the stationary state under study has definite parity, the expectation value \( \langle d \cdot J \rangle \) vanishes being the pseudoscalar product of a polar and an axial vector. Obviously, the existence of the EDM necessarily requires \( \mathcal{P} \)-violation.

However, this is not sufficient. The rotational scalar \( \langle d \cdot J \rangle \) cannot depend on the projection \( J_z \) of the atomic state; therefore it should have the same value for \( J_z = M \) and \( J_z = -M \). On the other hand, the transformation from \( M \) to \( -M \) is equivalent to time reversal, when \( J \) changes sign while \( d \) does not. Therefore the non-zero expectation value of any polar \( T \)-even vector requires, in addition, a violation of \( T \)-invariance (the classical Purcell-Ramsey theorem \[27\]). In contrast to that, the non-zero expectation values of \( \mathcal{P} \)-even \( T \)-odd vector operators, such as the magnetic moment, do not require any violation of fundamental symmetries. The arguments do not change in the presence of the hyperfine structure, one just needs to substitute the total angular momentum \( F = J + I \) instead of the atomic spin \( J \).

B. Schiff theorem

In order to see how the \( \mathcal{P}, T \)-violating hadronic forces induce the atomic EDM we consider (for simplicity, in the non-relativistic approximation) the Hamiltonian of the atomic system,

\[ H_{\text{atom}} = H_{\text{el}} + H_{\text{nucl}} + \sum_a e\phi(r_a), \]

(2)

where \( H_{\text{el}} \) and \( H_{\text{nucl}} \) are total Hamiltonians of interacting electrons and nucleons, respectively, while \( \phi(r) \) is the electrostatic potential generated by the nuclear ground state charge density \( \rho(x) \),

\[ \phi(r) = \int d^3x \frac{\rho(x)}{|r-x|}. \]

(3)

The EDM is probed by the external electric field \( E \) that interacts with electrons and protons,

\[ H_{\text{ext}} = -\left( e \sum_a r_a + \hat{D} \right) \cdot E, \]

(4)

where \( \hat{D} \) is the operator of the nuclear electric dipole moment. Due to \( \mathcal{PT} \)-violation, this operator can have a non-zero expectation value \( \langle D \rangle \) in the exact nuclear ground state.
In order to proceed with the calculation of the response of the system to the electric field, we follow the method of Refs. [32] (see the Appendix) and [33]. It is convenient to make a canonical transformation of the full Hamiltonian \( H = H_{\text{atom}} + H_{\text{ext}} \) using a unitary operator \( \hat{U} = \frac{\langle D \rangle}{Z|e|} \cdot \sum_a \hat{p}_a \).

We can limit ourselves to the first order with respect to the small quantities like \( \langle D \rangle \), so that

\[
H' = e^{i\hat{U}}He^{-i\hat{U}} \approx H + i[\hat{U}, H].
\]

The commutator in eq. (6) is given by

\[
i[\hat{U}, H] = \frac{1}{Z} \langle D \rangle \cdot (ZE + E_e),
\]

where

\[
E_e = -\sum_a \nabla_a \phi(r_a)
\]

can be interpreted as the electric field on the nucleus produced by atomic electrons. In a stationary state \( |\Psi\rangle \) of the full Hamiltonian \( H \),

\[
\langle \Psi |[\hat{U}, H]|\Psi \rangle = 0.
\]

This means that the stationary state in the external field polarizes the electron configuration in such a way that the total field acting on the nucleus vanish,

\[
ZE + \langle E_e \rangle = 0.
\]

This screening is the content of the Schiff theorem [34, 35]. In simple terms, in a stationary state, forces on the nuclear dipole are to be compensated. Now we need to consider what is left in the Hamiltonian after the canonical transformation (6).

The interaction of the external field with the nuclear dipole is mostly taken in account, except for the fluctuational term \(-(D - \langle D \rangle) \cdot E\). Therefore in the first order the external field does not lead to the energy shift (in higher orders it still influences the nuclear polarizability). The external field however renormalizes the electron-nucleus interaction: instead of the usual electrostatic potential \( \phi(r) \) we have now

\[
\phi'(r) = \phi(r) - \frac{1}{Ze} \langle D \rangle \cdot \nabla \phi(r).
\]
This is the starting point of the path that leads to the Schiff moment.

We have to mention that a different form of the canonical transformation,

$$\hat{U} = \frac{D}{|e|} \cdot \sum_a \hat{p}_a,$$

was considered recently [36]. Here the operator $\hat{D}$ is used, in contrast to its expectation value in our version [34]. The transformation (12), leading to the exact cancelation instead of our fluctuation term, brings instead the commutators of the operator $\hat{D}$ with the full nuclear Hamiltonian and therefore introduces complicated nuclear correlations. The derivation above is in agreement with previous results for the Schiff moment.

As indicated in the pioneering work by Schiff [34], the screening theorem is violated by the hyperfine interactions. Actually, this effect turns out to dominate in hydrogen and helium atoms [37]. However, in heavy atoms, which are subject of our main interest, the contribution of the Schiff moment (see the next subsection), together with the relativistic enhancement of the electronic wave functions in the vicinity of the nucleus, makes the situation much more promising.

C. Schiff moment

The standard expression for the Schiff moment [38] can be derived in many ways. If we neglect the relativistic corrections of the order $(Z\alpha)^2$ we can use a simple expansion of the nuclear charge density $\rho(r)$ in the series over gradients of the delta-function,

$$\rho(x) = \left\{ A + (B \cdot \nabla) + \frac{1}{2} C_{ik} \nabla_i \nabla_k + \ldots \right\} \delta(x).$$

A more precise derivation accounting for relativistic corrections can be found in [39, 40].

The coefficients of the expansion (13) are related to the nuclear multipole moments,

$$\int d^3 x \rho(x) = Z|e|,$$

$$\int d^3 x \rho(x)x = \langle D \rangle,$$

$$\int d^3 x \rho(x)(3x_i x_k - \delta_{ik} x^2) = Z|e|\langle Q_{ik} \rangle,$$

$$\int d^3 x \rho(x)x^2 = Z|e|\langle x^2 \rangle_{ch},$$

$$\int d^3 x \rho(x)x^2 x = \langle D^{(2)} \rangle,$$

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etc. The operator $D^{(2)}$ is associated with the isoscalar dipole giant resonance since the usual isoscalar dipole moment reduces to the center-of-mass excitation.

Expressing the charge density (13) in terms of physical multipoles, we obtain

$$\rho(x) = \sum_l \rho^{(l)}(x) \delta(x), \quad (19)$$

where the multipole operators $\rho^{(l)}$ acting on the delta-function are given by

$$\rho^{(0)} = Z|e| \left\{ 1 + \frac{1}{6} \langle x^2 \rangle_{\text{eh}} \nabla^2 + \ldots \right\}, \quad (20)$$

$$\rho^{(1)} = - \left( \langle D \rangle + \frac{1}{10} \langle D^{(2)} \nabla^2 \rangle \right) \cdot \nabla + \ldots, \quad (21)$$

$$\rho^{(2)} = \frac{Z|e|}{6} \langle Q_{ik} \rangle \nabla_i \nabla_k + \ldots \quad (22)$$

This expansion enters the effective potential $\phi'(r)$ of eq. (11) that, after taking the expectation value in the nuclear ground state $|0\rangle$, becomes

$$\langle 0 | e \phi'(r) | 0 \rangle = \frac{Ze^2}{r} + 4\pi e (S \cdot \nabla) \delta(r) + \ldots, \quad (23)$$

where $S$ is the expectation value of the Schiff moment vector operator,

$$\hat{S}_i = \frac{1}{10} \int d^3 x \rho(x) \left\{ x^2 x_i - \frac{5}{3} \langle x^2 \rangle_{\text{eh}} x_i - \frac{2}{3} \langle Q_{ik} \rangle x_k \right\}. \quad (24)$$

In addition, this operator can have contributions from the possible internal dipole moments of the nucleons. These contributions cannot be experimentally distinguished from those determined by the nuclear multipoles in eq. (24).

D. From nuclear Schiff moment to atomic EDM

The expectation value of the nuclear Schiff moment (24), similar to the atomic EDM (1), is given by the effective operator of the vector model for the nuclear ground state with spin $I > 0$,

$$\hat{S} = \frac{\langle S \cdot I \rangle}{I(I+1)} \hat{I}. \quad (25)$$

The exact nuclear state $|I\rangle$ should be a superposition of the ground state $|I; 0\rangle$ (found in the absence of weak interactions) and admixtures of the opposite parity states $|I; k\rangle$ induced by the $\mathcal{PT}$-violating weak interaction $W$,

$$|I\rangle = |I; 0\rangle + \sum_{k \neq 0} \frac{\langle I; k | W | I; 0 \rangle}{E_0 - E_k}. \quad (26)$$
The weak perturbation \[ (26) \] creates the non-zero expectation value of the Schiff moment,

\[
\langle S \rangle = 2 \text{Re} \sum_{k \neq 0} \frac{\langle I; 0|S|I;k \rangle \langle I;k|W|I;0 \rangle}{E_0 - E_k}.
\]  

(27)

The unknown \( \mathcal{P} \mathcal{T} \)-violating weak interaction \( W \), under the assumption of two-body nucleon-nucleon forces and to the first order in the nucleon velocities, can be parameterized as \[ (28) \]

\[
W_{ab} = \frac{G}{\sqrt{2}} \frac{1}{2m} \left\{ (\eta_{ab}\vec{\sigma}_a - \eta_{ba}\vec{\sigma}_b) \cdot \nabla_a \delta(x_a - x_b) 
+ \eta_{ab}'[\vec{\sigma}_a \times \vec{\sigma}_b][(\vec{p}_a - \vec{p}_b), \delta(x_a - x_b))]_+ \right\}.
\]

Here \( G \) is the Fermi constant of the weak interaction, \( m \) is the nucleon mass, while \( \vec{\sigma}_{a,b}, x_{a,b}, \) and \( \vec{p}_{a,b} \) are the spins, positions and momenta, respectively, of the interacting nucleons \( a \) and \( b \); \([,]_+ \) means an anticommutator. The dimensionless coupling constants, \( \eta_{ab} \) and \( \eta_{ab}' \), of the \( \mathcal{P}, \mathcal{T} \)-violating forces are to be extracted from the values of the atomic EDM. Theoretical arguments \[ 42, 43 \] show that such an interaction is determined mainly by the exchange of neutral pions.

The Schiff moment influences the atomic electrons through the second term of the potential \[ (23) \]; a more accurate account of the finite size of the nucleus can be found in Ref. \[ 39 \]. This mixes electron orbitals of opposite parity and generates the EDM of the atom. The result of detailed atomic calculations \[ 44 \] can be presented as the proportionality between the atomic EDM \( d \) and the Schiff moment \( S \), eq. \[ (27) \],

\[
d = \xi \left( \frac{S}{e \cdot \text{fm}^3} \right) 10^{-17} e \cdot \text{cm}.
\]  

(29)

The numerical factor \( \xi \) is the main result of complicated calculations, which can be a topic of a special review article. This factor grows with the nuclear charge reaching the values 3.3 for radon and -8.5 for radium.

E. Briefly on the experimental situation

As stated in the first line of Ref. \[ 29 \], “No permanent electric-dipole moment (EDM) of an elementary particle, atom, or molecule has yet been detected after several decades of experimentation”. We are interested here only in the experiments which are sensitive to the nuclear spin and Schiff moment. Presently the measurement of the atomic EDM is
pursued by several experimental groups, and we mention only few recent results based on various cutting-edge applications of methods of quantum optics. There exist also interesting suggestions for the EDM measurement in storage rings [45, 46, 47].

The data obtained for $^{129}$Xe and $^{199}$Hg provide the best available limits. The measurement [48] of the Zeeman splitting in parallel or antiparallel electric and magnetic fields with simultaneous presence of laser polarized $^{129}$Xe and $^3$He (the latter served as a “comagnetometer”) gave $d(^{129}$Xe) = $(0.7 \pm 2.8) \times 10^{-27}$ e cm. The upper boundary value for the EDM of $^{199}$Hg was given in Ref. [29] as $|d(^{199}$Hg)| < $8.7 \times 10^{-28}$ e·cm which was better by a factor of 25 than the previous mercury measurement [49]. The method of [29] employed the measurement of the spin precession in the electric field and had many technical improvements compared to [49]. The next step in the same direction was made by the same group at the University of Washington in Ref. [30]. By using a different technique of measuring the Zeeman precession of nuclear spins in parallel electric and magnetic fields, the limit for the EDM of $^{199}$Hg was lowered by the factor of 4 up to $|d(^{199}$Hg)| < $2.1 \times 10^{-28}$ e·cm. Already this limit puts stringent constraints on $\text{CP}$-violating effects beyond the standard model [30].

The results of the Berkeley experiment [50] performed on atomic $^{205}$Tl in the ground state with the use of the atomic-beam magnetic resonance and laser optical pumping improved the results of the previous attempts [51] and were interpreted as a limit for the electric dipole of the electron, $|d_e| \leq 1.6 \times 10^{-27}$ e cm. Essentially, here the signal of $\mathcal{P}, \mathcal{T}$-violation is given by the dependence on the $\mathcal{P}, \mathcal{T}$-odd relativistic invariant $(E \cdot B)$ of electromagnetic fields.

Isotopes of radium and radon seem to be the appropriate candidates for the combination of nuclear and atomic enhancement factors; we will discuss later more in detail the advantages of heavy nuclei with a combination of quadrupole and octupole deformation. Among these isotopes $^{225}$Ra is one of the most attractive due to its nuclear spin 1/2 and reasonably long lifetime $t_{1/2} = 15$ days. Specific near-degeneracies in the atomic spectrum can lead to further enhancements [44, 52]. Because of this importance, the success of the Argonne group [53] can be estimated as a sign of the serious progress in this direction. It turned out to be possible to perform laser trapping of $^{225}$Ra (as well as $^{226}$Ra) and to measure the isotope shift, hyperfine splittings and lifetimes of certain levels in cooled atoms. The thermal black-body radiation at room temperature served as an instrument in the redistribution of level populations.

Lighter radium and radon isotopes, which also could, as we discuss below, compete for
favorable Schiff moment conditions, were not sufficiently studied until now. They mostly have much shorter alpha-decay lifetime (only $^{223}$Ra has $t_{1/2} = 11$ days but nuclear spin $I = 3/2$ and the non-zero quadrupole moment that may lead to systematic errors in atomic experiments). The successful techniques of nuclear orientation of radon isotopes $^{209}$Rn and $^{223}$Rn by spin-exchange optical pumping was developed long ago [54]. An experiment to measure the atomic EDM of $^{223}$Ra is planned at TRIUMF (E-929 collaboration) with results expected in a number of years (the production rate of $^{223}$Rn at the ISAC facility is $10^7$/s). Also the KVI group is planning to study the EDM of laser-trapped radium isotopes, in particular of $^{225}$Ra. A more detailed information on the last two works, as well as about the experimental situation in general, can be found online in the presentations by T. Chupp and K. Jungman at the workshop at INT, Seattle, 2007 [55]. In the light of ideas of possible soft mode enhancement the pool of nuclear candidates can become wider. There are also ideas in the literature of using molecular and condensed matter systems with strong local electric fields [56, 57, 58] where experiments are under preparation, see for example, presentation by D. Budker [55].

III. SINGLE-PARTICLE SCHIFF MOMENT

Now we concentrate on the magnitude of the nuclear Schiff moment that results from complicated many-body dynamics in heavy nuclei. In the simplest meaningful approximation, the ground state of an odd-$A$ nucleus has one unpaired particle. In this picture the many-body dynamics is reduced to the mean field that defines the symmetry of single-particle motion. This is what is usually called nuclear shape [59]. Another important ingredient is the pairing interaction that introduces the seniority quantum number $v$ which can be identified with the number of unpaired particles. In this approximation $v = 0$ for the ground state of an even-even nucleus, and $v = 1$ in the odd-$A$ case.

The shape is defined with respect to the intrinsic (body-fixed) reference frame, see the conventional Fig. 1. This does not matter in the spherical case, when the mean field and spin-orbit coupling generate single-particle orbitals with definite angular momentum $j = l+s$ and degeneracy with respect to the arbitrarily chosen projection $j_z = m$. However, in the deformed case, the reference frame is rotating together with the body, and this rotational motion defines the orientational wave function $D_{MK}^I$, where $I$ and $I_z = M$ are total nuclear
FIG. 1: The intrinsic shape corresponding to the axially symmetric combination of quadrupole and octupole deformation; parameters are $\beta_2 = 0.3$ and $\beta_3 = 0.1$; the angular momentum vector $I$ has the body-fixed projection $K$ and the space-fixed projection $M$.

spin and its projection onto the laboratory quantization axis. Here and below we assume that the shape has axial symmetry characterized by the unit vector $n$ and one can define the conserved component $(I \cdot n) = K$ of the total spin along the symmetry axis. The single-particle states in this case are Nilsson orbitals with a certain angular momentum projection $j_z = \kappa$. Due to time-reversal invariance of strong forces, the orbitals $\pm \kappa$ are degenerate ($Kramers theorem$). The presence of deformation of various multipolarities is an important resource in search for the enhancement of violation of fundamental symmetries.

In the body-fixed frame there are no angular momentum restrictions, and any multipole operator, including the Schiff moment, can have a non-zero intrinsic value. The observable
value of $S$ in the space-fixed frame appears only due to the mixing induced by the weak interaction. It is believed that the main contribution comes from the coherent mean-field part of the interaction (28) that can be written as a one-body operator,

$$
\mathbf{W}(x) = \frac{G}{\sqrt{2}} \frac{1}{2m} \frac{n}{4\pi} (\vec{\sigma} \cdot \nabla) \rho(x),
$$

where $\rho(x)$ is the nuclear density. In the single-particle approximation, the weak interaction mixes orbitals of opposite parity; in the spherical case they have $j^\prime = j$ but different orbital momenta, $l^\prime = l \pm 1$.

Rare accidental proximity of the orbitals of opposite parity can lead to the small energy denominators in (27). However, for single-particle mixing, this can hardly enhance the outcome since the matrix elements of $\mathbf{W}$, eq. (30), are roughly proportional to those of the single-particle momentum operator, and therefore to the energy differences of the mixed orbitals. This cancels the small energy denominators.

The next step beyond the single-particle model should account for the residual interaction (pairing is in a sense a part of the mean-field picture). Realistic calculations were performed in various versions of configuration mixing. The main effect appearing here is the core polarization by the unpaired particle. The quasiparticles are dressed by this polarization and all observables are renormalized. In agreement with the previous experience, the renormalization can lead to qualitatively new results if there exist low-lying collective modes of considerable strength. But we do not know about significant collective dipole strength in the vicinity of the ground state. Because of this absence of coherence, the results of such calculations for the Schiff moment differ from pure single-particle estimates not more than by the factor of about 2.

IV. STATIC DEFORMATION

We have to search for specific structural features which can bring closely such levels of opposite parity that can have a large probability of being mixed by the interaction $W$. These features are related to the possible coherence of mixing that involves collective contributions of many particles. The main attempts in this direction use deformed nuclei as the appropriate arena for the combined action of intrinsic symmetry and weak interactions.
A. Combination of quadrupole and octupole deformation

Let us consider an axially symmetric deformed odd-$A$ nucleus. The deformed mean field spontaneously breaks rotational symmetry. In the usual approximation, the nuclear rotation (which plays the role of the Goldstone mode that restores the proper quantum numbers of angular momentum) is adiabatic with respect to intrinsic excitations. The full wave function can be presented as the product of the rotational Wigner function $D_{MK}^I$ depending on the orientational angles and the intrinsic function $\chi_K$, where $K$ is an intrinsic pseudoscalar. In the body-fixed frame, any polar vector, such as the Schiff moment $S$, can have a non-zero expectation value $S_{\text{intr}}$ without any $\mathcal{P}$- or $\mathcal{T}$-violation. The symmetry dictates the direction of this vector along the symmetry axis,

$$S_{\text{intr}} = S_{\text{intr}} n.$$

(31)

However, this intrinsic vector is averaged out by rotation because the only possible combination in the space-fixed frame is again similar to the one we have seen in eqs. (1) and (25), namely proportional to the pseudoscalar product $\langle (n \cdot I) \rangle$ that violates $\mathcal{P}$- and $\mathcal{T}$-invariance. If the $\mathcal{P}$, $\mathcal{T}$-violating forces create an admixture $\alpha$ of states of the same spin and opposite parity, the average orientation of the nuclear axis arises. In the linear approximation with respect to $\alpha$,

$$\langle (n \cdot I) \rangle = 2\alpha K,$$

(32)

and, therefore, we acquire the space-fixed Schiff moment (25) along the laboratory quantization axis,

$$\langle IM|\hat{S}|IM \rangle = S_{\text{intr}} \frac{2\alpha K M}{I(I+1)}.$$

(33)

Now the idea is to obtain a large intrinsic Schiff moment and not to lose much in translating the result to the space-fixed frame.

In order to have a significant value of the intrinsic Schiff moment, it is not sufficient to have a standard quadrupole deformation: we need a type of deformation that distinguishes two directions of the axis violating the symmetry with respect to the reflection in the equatorial plane perpendicular to the symmetry axis. The collective effect sought for may be related to the simultaneous presence of quadrupole and octupole deformation, the latter creating a pear-shaped [65, 66] (or even a heart-shaped [67]) intrinsic mean field. The importance of octupole deformation for the transmission of statistical parity violation through intermediate
stages of the fission process was understood long ago \[17\]; this possibility was also considered in Ref. \[68\] in relation to the “sign problem” (predominance of neutron resonances with the same sign of $\mathcal{P}$-violating asymmetry in $^{232}$Th that seemingly contradicts to the statistical mechanism of enhancement). Now we need the octupole deformation in the ground state.

In the phenomenological collective description of nuclear deformation in terms of the equipotential surfaces,

$$R(\theta) = R \left[ 1 + \sum_{l=1}^{\infty} \beta_l Y_{l0}(\theta) \right], \quad (34)$$

the vector terms, $l = 1$, emerge, after excluding the center-of-mass displacement, through bilinear combinations of even and odd multipoles,

$$\beta_1 = -\sqrt{\frac{27}{4\pi}} \sum_{l=2}^{\infty} \frac{l+1}{(2l+1)(2l+3)} \beta_l \beta_{l+1}. \quad (35)$$

The main contribution that comes from the product of the lowest static multipoles, quadrupole and octupole, determines the collective intrinsic Schiff moment \[32, 69\],

$$S_{\text{intr}} \approx \frac{9}{20\sqrt{35\pi}} eZ R^3 \beta_2 \beta_3. \quad (36)$$

The collective character of the octupole moment leads to the strong enhancement of the intrinsic Schiff moment compared to the single-particle estimates. Of course, the results are sensitive to the details of the nuclear models, mean field and effective interactions, but, within a factor of about 2, the Schiff moment may be enhanced up to two to three orders of magnitude \[32, 69, 70\].

Such results were obtained under an assumption of close levels of opposite parity mixed by the interaction $W$, with the splitting $\Delta = |E_+ - E_-| \approx 50$ keV. This is a real situation in $^{225}$Ra ($\Delta = 55$ keV, $I = 1/2$) and in $^{223}$Ra ($\Delta = 50$ keV, $I = 3/2$). The radium and radon isotopes seem to be promising because of clear manifestations of octupole collectivity.

In addition, the large nuclear charge is favorable for the enhancement of the atomic EDM \[71\]. We need to note that the resulting space-fixed expectation value of the Schiff moment, according to eqs. (33) and (36), is proportional to the product $\alpha S_{\text{intr}}$ and therefore to $\beta_3^2$.

### B. Parity doublets

The mixing can be particularly enhanced if the admixed states are parity doublets \[32, 65, 66, 68, 69\]. In the presence of the octupole deformation (or for any axially symmetric
shape with no reflection symmetry in the equatorial plane), the states of certain parity Π are even and odd combinations of intrinsic states χ±K with the quantum numbers ±K ≠ 0. The intrinsic wave functions which differ just by the “right” or “left” orientation of the pear-shape configuration should be combined in the states with definite parity Π,

\[ |IMK; Π\rangle = \sqrt{\frac{2I + 1}{8\pi}} \left[ D^I_{MK}χ_K + Π(-)^I+KD^I_{M−K}χ−K \right]. \] (37)

Such doublets in fact do not even require axial symmetry; the label ±K may have a more general meaning. The intrinsic partners are time-conjugate and, according to the Kramers theorem, they are degenerate in the adiabatic approximation. In the non-axial case, one can write the wave function as a sum over K of items similar to those in eq. (37).

In reality the doublets (13) are split by additional interactions. This can be accomplished

by Coriolis forces (the body-fixed frame of the rotating nucleus is non-inertial) or by the tunneling between the two orientations. However such a splitting is not large and the similarity of intrinsic structure should help in increasing the mixing by the weak interactions. As explained in Refs. [16, 32, 65, 68, 69], only the interaction violating both \(P\)- and \(T\)-invariance can mix the doublet partners because

\[ \langle IMK; −Π|W|IMK; Π\rangle = \frac{1}{2}[\langle χ_K|W|χ_K\rangle − \langle χ−K|W|χ−K\rangle]. \] (38)

The matrix elements of the pseudoscalar \(W\) change sign together with \(K\) which is possible only if the time-reversal invariance is violated, along with parity. The “normal” weak interaction is \(T\)-invariant. Therefore it is capable of mixing the parity doublets only with the help of a mediator, a regular \(P, T\)-conserving interaction, including that one responsible for the doublet splitting. This indirect mixing of parity doublets was suggested in Ref. [68] for explaining the “sign problem” in \(^{232}\)Th. In contrast to this, the \(P, T\)-violating interaction can mix the parity doublets directly, which is important for the enhancement of the Schiff moment.

The big enhancement predicted in this situation is illustrated by the results of calculation given in Ref. [32], see table (39). We select here the cases where the energy splitting \(ΔE\) between the partners of the parity doublet is experimentally known. The parameter \(η\) is defined in eq. (30).
|             | $^{223}\text{Ra}$ | $^{225}\text{Ra}$ | $^{221}\text{Fr}$ | $^{223}\text{Fr}$ | $^{225}\text{Ac}$ | $^{229}\text{Pa}$ |
|-------------|------------------|------------------|------------------|------------------|------------------|------------------|
| $\Delta E_{\exp}$ (keV) | 50               | 55               | 234              | 161              | 40               | 0.2              |
| $S_{\text{intr}}$ (e fm$^3$) | 24               | 24               | 21               | 20               | 28               | 25               |
| $S(10^8(\eta e \text{ fm}^3)$ | 400              | 300              | 43               | 500              | 900              | 12000            |
| $D(10^{25}(\eta e \text{ cm})$ | 2700             | 2100             | 240              | 2800             |                  |                  |

The last line contains the results of atomic calculations which can be in fact extrapolated \[32\] from the work for lighter atomic analogs \[72\].

V. SOFT OCTUPOLE MODE

As was mentioned earlier, in a nucleus with the combination of developed quadrupole and octupole deformations, the intrinsic Schiff moment is determined by the collective octupole moment $\beta_3$, whereas the Schiff moment in the space-fixed frame is proportional to its square. Obviously, the sign of the octupole moment is not important. This gives rise to the idea \[73, 78\] that, instead of static octupole deformation, the same role of the enhancing agent can be played by the dynamic octupole deformation.

The soft octupole mode (low-lying collective $3^-$ “one-phonon” state) is observed in many nuclei and, for a small frequency $\omega_3$ of this mode, the vibrational amplitude increases, $\langle \beta_3^2 \rangle \propto 1/\omega_3$. This relation would be precise for the harmonic vibrations; its quadrupole analog sometimes is called the Grodzins relation \[74\]. In practice it approximately works although octupole vibrations are in many cases noticeably fragmented and reveal anharmonicity \[75, 76\]. If the Schiff moment is indeed enhanced under such conditions without static octupole deformation, this can provide a more broad choice for the experimental search. Numerically, the mean square amplitude $\langle \beta_3^2 \rangle$ is close to the squared value $\langle \beta_3 \rangle^2$ of static octupole deformation in pear-shaped nuclei. This value can be extracted from the reduced transition probability $B(E3; 0^+ \rightarrow 3^-)$, see the compilation in \[77\].

In the presence of the soft octupole mode, the octupole moment $Q_{3\mu}$ oscillates with the low frequency, and its intrinsic component along the axis defined by the static quadrupole deformation $\beta_2$ is phenomenologically given by

$$Q_3 = \frac{3}{4\pi} e Z R^3 \beta_3. \quad (40)$$
This implies, eq. (36), the slowly oscillating intrinsic Schiff moment,

\[ S_{\text{intr}} = \frac{3}{5 \sqrt{35}} Q_3 \beta_2 \]  

(as we have already stressed, the intrinsic Schiff moment does not depend on violation of fundamental symmetries).

Now we need to introduce the mechanisms converting the intrinsic Schiff moment into observable \( P, T \)-violating effects. The description of the previous paragraph referred to the deformed even-even core. The space-fixed Schiff moment needs the non-zero nuclear spin so we proceed to the neighboring odd-\( A \) nucleus. The unpaired nucleon interacts with the octupole mode. This dynamic octupole deformation of the mean field can mix, still in the body-fixed frame, the single-particle orbitals of opposite parity. As suggested in Ref. [78], the mixing leads to the non-vanishing expectation value of the weak interaction \( \langle W \rangle \) in the body-fixed frame. This process can be called “particle excitation”. In a parallel process of “core excitation” [79], the octupole component of the weak \( P, T \)-violating field of the odd particle can excite the soft octupole mode in the core.

The estimate of the first mechanism can be based on the octupole-octupole part of the residual nucleon interaction. The original orbital \( |\nu\rangle \) acquires the octupole phonon admixture while the particle is scattered to some orbitals \( |\nu'\rangle \) of opposite parity,

\[ |\nu\rangle \Rightarrow |\tilde{0}\rangle = |\nu; 0\rangle + \sum_{\nu'} a_{\nu'} |\nu'; 1\rangle, \]  

where the number after the semicolon in the state vector indicates the number of octupole phonons. The orthogonal one-phonon state is, in the same approximation,

\[ |\nu; 1\rangle \Rightarrow |\tilde{1}\rangle = |\nu; 1\rangle + \sum_{\nu'} b_{\nu'} |\nu'; 0\rangle. \]  

The mixing amplitudes between the orbitals with energies \( \epsilon_\nu \) are

\[ a_{\nu'} = \frac{\beta_3 (F_3)_{\nu' \nu}}{\epsilon_\nu - \epsilon_{\nu'} - \omega_3}, \quad b_{\nu'} = \frac{\beta_3 (F_3)_{\nu' \nu}}{\epsilon_\nu - \epsilon_{\nu'} + \omega_3}, \]  

where we assume the octupole forces in the form \( \beta_3 F_3 \), the octupole collective coordinate \( \beta_3 \) being defined by eq. (40), while \( F_3 \) is an operator acting on the particle and having the form close to \( -(dU/dr) Y_{30} \) with the radial factor usually taken as a derivative of the spherical mean field potential, a reasonable approximation for realistic deformations of low
multipolarities. The quantity $\beta_3$ in eq. (44) is the transition matrix element of this collective octupole coordinate between the ground and one-phonon states in the even-even core.

Now the states $|\tilde{0}\rangle$ and $|\tilde{1}\rangle$ are mixed by the $P, T$-violating potential. This mechanism involves the coherent part of the weak interaction $\overline{W}$ averaged over the core nucleons. The mixing matrix element is found as

$$\langle \tilde{0}|\overline{W}|\tilde{1}\rangle = \beta_3 \sum_{\nu} \frac{2(\epsilon_\nu - \epsilon_{\nu'})}{(\epsilon_\nu - \epsilon_{\nu'})^2 + \omega_3^2} W_{\nu\nu'}(F_3)_{\nu\nu'},$$

which is still an operator linear in the collective coordinate $\beta_3$. In the adiabatic limit, when the octupole mode frequency $\omega_3$ is small compared to the single-particle spacing between the orbitals of opposite parity, the weak interaction is essentially acting at a fixed octupole deformation and then it is averaged over the slowly evolving phonon wave function. The result practically coincides with that for the static octupole deformation discussed earlier. The only difference is the substitution of the static $\beta_3^2$ by the dynamic mean square average $\langle \beta_3^2 \rangle$.

In the core excitation mechanism [73], the effective part of the weak interaction $W_{ab}$ acts between the valence nucleon $b$ and the paired nucleons $a$ in the core. Because of pairing in the core, only the contribution proportional to the spin of the valence nucleon survives,

$$W_{ab} = -\frac{G}{\sqrt{2}} \frac{1}{2m} \eta_{ba} \left( \nabla_a \cdot \psi_b^\dagger (r_a) \vec{\sigma}_b \psi_b (r_a) \right).$$

We need to extract from this interaction the octupole component $W_3$ proportional to the operator $Q_3 = r^3 Y_{30}$. The result [73] depends on the specific orbital of the external nucleon and can be presented in the form

$$(W_3)_a \approx k \frac{G}{m R^7} Q_3 \eta_{ba}$$

(this operator has to be multiplied by the creation or annihilation operator of the $3^-$ phonon). Here $k$ is the numerical factor determined by the spin-orbit structure of the valence orbital; in typical cases $|k| \approx 0.6$. The matrix element of this interaction exciting an octupole phonon (that contains both proton and neutron coherent components) is given by

$$\langle 1|W_3|0\rangle = k \frac{G}{m R^7} AR^3 \frac{3}{4\pi} \langle \beta_3 \rangle^2 \eta_b,$$

where the coupling constant is $\eta_b = (Z/A)\eta_{bp} + (N/A)\eta_{bn}$, and the subscript $b$ is $n(p)$ for the odd neutron (proton).
Using the mixing produced by the operator $W_3$ for calculating the effective Schiff moment operator and projecting to the space-fixed frame we come to the result of the same order of magnitude as in the case of the particle excitation. Compared to the static octupole deformation, the difference is, apart from numerical factors of order one, just in the substitution of static $\beta_3^2$ by the effective dynamic mean square value. Taking the limiting value in $^{199}\text{Hg}$ as a current standard, we can expect the enhancement in the interval of 100 - 1000 if the energy spacing $\Delta$ is of the order or less than 100 keV. The appropriate candidates are $^{223,225}\text{Ra}$, $^{223}\text{Rn}$, $^{223}\text{Fr}$, $^{225}\text{Ac}$, and maybe $^{239}\text{Pu}$, where the estimates of Ref. [73] are lower than in Ref. [78].

VI. SOFT QUADRUPOLE AND OCTUPOLE MODES

A. RPA approach

The results of the previous consideration point out a tempting possibility of searching for the significant enhancement of the Schiff moment in a broader class of spherical nuclei where both collective modes, quadrupole and octupole, are clearly pronounced and have low frequencies. As an example, one can mention light spherical isotopes of radium and radon. The experimental data [79] for $^{218,220,222}\text{Rn}$ and for other even-even nuclei in this region show long quasivibrational bands of positive and negative parity, where the energy intervals do not obey the rotational rules. The phonon frequencies are quite low, and the strong E1 transitions are observed between the appropriate members of the quadrupole and octupole bands. The softness of the modes and large phonon transition probabilities $B(E2; 0^+ \rightarrow 2^+)$ and $B(E3; 0^+ \rightarrow 3^-)$, along with strong dipole interband coupling, indicate that the situation might be favorable for the enhancement of the Schiff moment.

The mixing of the $2^+$ and $3^-$ phonons with the valence particle in a neighboring odd-$A$ nucleus can be considered as a slow (adiabatic) process of adjustment of the valence orbitals to the oscillating mean field, as we argued in the previous section. If the particle can form states with the same spin in both types of mixing, these states should be rather close in energy and can be mixed among themselves by the weak interaction. Here we do not introduce any body-fixed frame so the angular momentum must be strictly conserved in those mixing processes. Thus, in our main eq. (27), we can have in the odd nucleus states
of both parities with the same \( I, M \) quantum numbers like

\[
| IM \rangle = \left[ C_0 \alpha_j^\dagger \delta_{jI} + \sum_{\lambda j'} C_2 (j' \lambda; I) (\alpha_j^\dagger Q_{\lambda'}^I) | 0 \rangle \right].
\]  

Here \( \alpha_{jm} \) and \( Q_{\lambda \mu} \) are quasiparticle and phonon operators, respectively, coupled in the second term of eq. (49) into correct total angular momentum \( I \), whereas \( | 0 \rangle \) represents the ground state of the even nucleus.

The detailed microscopic calculations along these lines were performed in Ref. [80]. In the neutron-odd nucleus, the proton contribution needed for the Schiff moment comes from the transition matrix element of the Schiff operator between the appropriate states (49) of the same spin \( I \) and opposite parity,

\[
\langle I^\pm, M = I | S_z | I^\mp, M = I \rangle = \sum_{\lambda \lambda' j} X(jI; \lambda \lambda') C_2 (j \lambda; I^\pm) C_2 (j \lambda'; I^\mp) (\lambda || S || \lambda').
\]  

where \( X(jI; \lambda \lambda') \) are geometric coefficients resulting from vector coupling of angular momenta. The reduced matrix element of the Schiff momentum, \( (\lambda || S || \lambda') \), is taken between the phonon states of opposite parity in the even-even core. Because of the strong dipole coupling between the corresponding bands found in the candidate nuclei, we expect that this matrix element should enhance the Schiff moment.

Concrete calculations [80] used the random phase approximation (RPA) in the form of the quasiparticle-phonon model [81]. The multipole-multipole forces are fixed in even nuclei by the phonon parameters. The result for the Schiff moment can be expressed in terms of the single-particle Schiff matrix elements, \( (j_1 || S || j_2) \), standard pairing amplitudes, \( (u, v) \), and the RPA phonon amplitudes of two-quasiparticle and two-quasihole components, \( (A, B) \),

\[
(\lambda || S || \lambda') = \sqrt{35} \sum_{123} (u_1 u_2 - v_1 v_2) \left\{ \begin{array}{ccc} \lambda & \lambda' & 1 \\ j_1 & j_2 & j_3 \end{array} \right\} 
\times (j_1 || S || j_2) [A_\lambda (23) A_{\lambda'} (31) + B_\lambda (23) B_{\lambda'} (31)].
\]  

The weak interaction was taken in the mean-field form, eq. (30),

\[
W_b(r) = \frac{G}{\sqrt{2}} \frac{1}{2m} \frac{1}{\eta(\vec{r} \cdot \vec{r})} \frac{1}{4 \pi r} \frac{d\rho(r)}{dr},
\]  

where \( \rho(r) \) is determined by the pairing occupancy factors in the core. There are several contributions of the interaction (52) to various parts of the complicated calculation: wave
functions of the unpaired quasiparticle, matrix elements of quasiparticle-phonon coupling, intermediate particle and phonon propagators, and phonon loops. Combining these calculations with the energy denominators we come to the final results.

At this stage we could not find an enhancement of the nuclear Schiff moment. For example, for the $^{219}$Rn isotope the matrix element of the weak interaction equals $-1.3 \, \eta \cdot 10^{-2}$ eV, and the final value of the ground state Schiff moment was $0.30 \, \eta \cdot 10^{-8} \, e \cdot fm^3$. Typically, the reduced matrix elements $(2^+|S|3^-)$ in the even nucleus are of the order $(1-2) \, e \cdot fm^3$, and the matrix elements of the Schiff operator between the ground state in the odd nucleus and its parity partner are around $0.1-0.2 \, e \cdot fm^3$. Final results for the Schiff moment are of the same order as in pure single-particle models (the single-particle contribution unrelated to the soft modes $^{[61, 62, 63]}$ has to be added).

These calculations seemingly contradict the idea of a possible enhancement by soft collective modes. Nevertheless, a useful exercise $^{[80]}$ confirms that the effect indeed exists but, in the RPA framework, requires artificially low collective frequencies when the dynamic deformation amplitudes increase as $\beta \propto 1/\omega$. One can consider the theoretical RPA limit of collapsing frequencies,

$$ \omega_{2,3} = y \omega_{2,3}, \quad y \ll 1, \quad (53) $$

and accurately separate the singular part of the RPA solutions. As the collective frequencies go down, the reduced matrix element $(2^+|S|3^-)$ in the even nucleus, the mixing matrix element of the weak interaction in the odd nucleus and the final Schiff moment grow large. These trends are seen in the following table $(54)$,

| Nucleus | $y$ | $(2^+|S|3^-)$ m.e. | $W$ m.e. | $S$ m.e. | $S$ |
|---------|-----|-------------------|----------|----------|---|
| $^{219}$Ra | 1   | 1.7               | -1.3     | -0.1     | 0.3  |
|          | 0.1 | 20                | 1.1      | -0.2     | -0.2 |
|          | 0.01| 195               | 53       | -0.2     | 6.2  |
| $^{221}$Ra | 1   | 2.2               | 0.2      | -0.2     | -0.1 |
|          | 0.1 | 23                | -19      | -0.5     | 6    |
|          | 0.01| 235               | -253     | -2.7     | 560  |

It is clear from the table that the matrix element $(2^+|S|3^-)$ indeed increases $\propto 1/\omega$. Other matrix elements are also sensitive to the level spacing in the odd nucleus. Here we need to mention that the RPA results with the parameters fitted to the phonon frequencies do not
produce a satisfactory description of entire spectra in odd nuclei.

**B. Going beyond RPA**

To summarize the findings of the previous subsection, in the situation when the phonon-quasiparticle coupling becomes strong, the standard RPA approach that accounts for a single-phonon admixture to quasiparticle wave functions, is not adequate. The effect of enhancement appears either with static deformation or in the strong coupling limit when effectively the condensate of phonons emerges that mimics the deformed field. In the exactly solvable particle-core model [82] with the soft monopole mode, $\lambda = 0$, the ground state of the odd-$A$ nucleus contains a coherent phonon state with the average number of phonons defined by the coupling constant. The quasiparticle strength in this regime is strongly fragmented over many excited states. Similar effects should take place for quadrupole and octupole modes [83, 84, 85] when the coherence finally leads to the phase transition to static deformation.

In agreement with above arguments, the calculations [80] with artificially quenched frequencies show that the wave function of the odd nucleus becomes exceedingly fragmented. For example, in the realistic case, $y = 1$, for the ground state $I = 7/2$ in $^{219}$Ra, there exists only one large combination of amplitudes required for the mixing, namely there are particle-phonon states $7/2^+$ with the wave function $(2g_{9/2}, 2^+)_7/2$ and $7/2^-$ with the wave function $(2g_{9/2}, 3^-)_7/2$; their weights in the full RPA wave functions are 98% for negative parity but only 8% for positive parity. With quenching of frequencies, these amplitudes are getting drastically reduced, up to 2% for negative parity and 1% for positive parity. Only after the spreading of the single-particle strength reached saturation in the orbital space under consideration, one can indeed see the enhancement of the Schiff moment.

Thus, the conventional RPA ansatz for the wave function of the odd nucleus as a superposition of particle+phonon components is invalid under conditions of soft collective modes. Many-phonon components take over a large fraction of the total wave function. Moreover, soft modes become mutually correlated. The correlation between soft quadrupole and octupole excitations was suggested in the global review of octupole vibrations [76]. The presence of the octupole phonon singles out the intrinsic axis (similar to the static deformation illustrated by Fig. 1) and triggers the *spontaneous breaking of rotational symmetry* with
an effective quadrupole condensate emerging. This mechanism follows from the simplest construction of the phenomenological coupling between the octupole and quadrupole modes that accounts for parity and angular momentum conservation. The effective Hamiltonian of this type is given by

\[ H = H_2 + H_3 + H_{23}, \]  

(55)

where \( H_2 \) and \( H_3 \) describe quadrupole and octupole collective modes (in principle including their anharmonicity). The interaction described by the destruction and creation operators \( d_\mu, d_\mu^\dagger \) and \( f_\mu, f_\mu^\dagger \), for the quadrupole and octupole phonons, respectively,

\[ H_{23} = x \sum_\mu \left[ (f^\dagger f)_\mu d_\mu^\dagger + \text{h.c.} \right], \]  

(56)

generates the equation of motion

\[ [d_\mu, H] = \omega_2 d_\mu + x(f^\dagger f)_\mu, \]  

(57)

where \( \omega_2 \) is the quadrupole frequency and \( x \) the coupling constant. In the presence of the octupole phonon, we obtain the quadrupole condensate,

\[ \langle d_\mu \rangle = -\frac{x}{\omega_2} \langle (f^\dagger f)_\mu \rangle, \]  

(58)

with the coherent intensity inversely proportional to the frequency as a characteristic feature of the situation associated with soft modes.

The direction of the effective self-consistent deformation is arbitrary, and, to restore the symmetry and appropriate quantum numbers of total nuclear spin in the space-fixed coordinate frame, we accept that the orientation of the deformation is given by a spherical function of corresponding rank,

\[ \langle d_\mu \rangle = \delta_2 \sqrt{\frac{4\pi}{5}} Y_{2\mu}^*(n), \quad \langle f_\mu \rangle = \hat{f} \sqrt{\frac{4\pi}{7}} Y_{3\mu}^*(n). \]  

(59)

Here \( n \) is the unit vector of the symmetry axis considered as a variable in the collective space. A similar operator approach was used long ago in the derivation of the nuclear moment of inertia without applying a cranking model \(^87\). The number \( N_3 = \sum_\mu f_\mu^\dagger f_\mu = \hat{f}^\dagger \hat{f} \) of octupole phonons is conserved by the Hamiltonian \(^{56} \), \( N_3 = 1 \) in the lowest \( 3^- \) state, and \( \hat{f}^\dagger \) is the operator generating the octupole vibrational mode in the body-fixed frame defined
by the orientation \( n \). Then eq. (58) equates the \( n \)-dependence and, with the ansatz (59), provides the effective quadrupole deformation parameter \( \delta_2 \),

\[
\delta_2 = -\frac{x}{\omega_2} \sqrt{5} \left( \begin{array}{ccc} 3 & 3 & 2 \\ 0 & 0 & 0 \end{array} \right) = -\sqrt{\frac{4}{21}} \frac{x}{\omega_2}.
\] (60)

The equation of motion for the octupole mode, given by the commutator \([f_\mu, H]\) and the effective quadrupole parameter (60), is linear. It relates the excitation energy \( E_3 \) of the octupole phonon with the corresponding unperturbed energy \( \omega_3 \) and the quadrupole condensate (60). Collecting again the terms expressing the angular dependence, we obtain

\[
E_3 = \omega_3 - \frac{8}{21} \frac{x^2}{\omega_2^2}.
\] (61)

This simple regularity [76] provides a clear correlation between the two modes. Recent measurements for the long chain of even-even xenon isotopes [86] show precisely such a correlation, with a rather large magnitude for the parameter \( x \) that exceeds the expectations for the anharmonic mode-mode coupling based on the standard RPA estimates.

A similar effect of condensation is brought in by the odd particle. The effective particle-phonon interaction is linear in phonon operators and proportional to different components of the particle density matrix

\[
\rho_{j_1m_1; j_2m_2} = \langle a^\dagger_{j_2m_2} a_{j_1m_1} \rangle = \sum_{L,\Lambda} (-)^{L-\Lambda+1-j_2-m_2} \begin{pmatrix} j_1 & L & j_2 \\ m_1 & -\Lambda & -m_2 \end{pmatrix} \rho_L(j_1j_2) Y^*_\Lambda(n).
\] (62)

in terms of the operators of creation, \( a^\dagger_{jm} \), and annihilation, \( a_{jm} \), of the particle in the spherical basis. Here the even-\( L \) parts come from the pairs of levels \((j_1, j_2)\) or \((j'_1, j'_2)\) of the same parity, whereas the odd-\( L \) ones correspond to the combinations \((j_1, j'_2)\) and \((j'_1, j_2)\) of single-particle levels of opposite parity. The equations of motion for phonons in the odd nucleus bring in their coherent states signaling the onset of an effective deformation, now for both, quadrupole and octupole modes. Self-consistently, the unpaired particle occupies the Nilsson-type orbitals in the deformed field characterized by the parameters \( \beta_2 \) and \( \beta_3 \) determined by the coupling constants with the particle and proportional to \( 1/\omega_2 \) and \( 1/\omega_3 \), respectively.

The operator \( S_{1\nu} \) of the Schiff moment in the even nucleus has a reduced matrix element \( S^0 \equiv \langle 2^+| S_1 |3^- \rangle \) between the low-lying \( 2^+ \) and \( 3^- \) states. As mentioned earlier, the dipole transitions between the states of the quadrupole and octupole bands are empirically known
to be enhanced in nuclei of our interest, such as light radium and radon isotopes \[79\]. The collective contribution to this operator can be written in terms of our phonon variables as

\[ S_{1\nu} = S^0 \sum_{\mu \mu'} (-)^{\nu + \mu} \begin{pmatrix} 1 & 2 & 3 \\ -\nu & -\mu & \mu' \end{pmatrix} \left( d_{\mu}^\dagger f_{\mu'} + (-)^{\mu + \mu'} f_{-\mu'}^\dagger d_{-\mu} \right). \]  

(63)

With the ground state expectation values of the effective deformation parameters in the odd nucleus, this gives a rotational operator

\[ \frac{S_{1\nu}}{S^0} = -\frac{1}{\sqrt{\pi}} \beta_2 \beta_3 Y_{1\nu}^* \]  

(64)

enhanced by small collective frequencies. As a result, we reduce the whole problem to that of the particle + rotor type \[32, 88\], where the static deformation is substituted by the effective deformation coming from the soft quadrupole and octupole modes of the spherical even core. The observable Schiff moment in the laboratory frame can come only from explicitly acting with the \( P \)- and \( T \)-violating weak interaction \( W \) that creates an admixture of the states \( |n\rangle \) having opposite parity to the ground state \( |0\rangle \) but the same spin \( I \).

In this spirit, a model of two single-particle levels of the same large \( j \) and opposite parity with \( n \) particles interacting through pairing and multipole-multipole (quadrupole and octupole) forces in the presence of the \( P \), \( T \)-violating weak interaction was considered using the exact diagonalization instead of the RPA \[89\]. The model does not introduce the intrinsic frame and preserves exact quantum constants of motion at all stages of calculation. The orbital space of the model is not large enough to demonstrate the constructive mutual support of the two soft modes; instead they compete for available quasiparticle excitations. Nevertheless, the model reveals the existence of a parameter region, where both frequencies in the even-even system are sufficiently low, while, in the neighboring odd system, matrix elements of the weak interaction and of the Schiff moment are significantly enhanced. One also clearly sees the appearance of parity doublets at a small spacing in the same parameter region. This set of conditions is favorable for a strong enhancement of the expectation value of the Schiff moment. The realistic calculations in the future will show how reliable is this evaluation.
C. Nuclear structure aspects

The consideration of mechanisms responsible for possible enhancement of violation of fundamental symmetries in many-body systems, such as atomic nuclei, elucidates also the problems of our understanding of nuclear structure and our ability to develop corresponding realistic theories. The statistical mechanism related to the uniform structure of compound states at high level density is in general understood. Even if it is impossible to calculate the properties of each individual state, we have sufficient knowledge of typical regularities, and in the region of quantum many-body chaos all states within a certain energy window “look the same” [21, 90]. The situation is different near the ground state, in the region important for the search of the atomic EDM.

As we have tried to argue, the low-lying collective modes and strong interaction between them and with quasiparticle excitations may lead to the strong enhancement of the effects we are interested in. Unfortunately, current microscopic nuclear structure theory does not give a clear answer to the question of the realistic strength of required interactions and their compatibility with the standard picture of nuclear shells. The two main obstacles in this direction are the necessity of large orbital space (we are looking at heavy nuclei) and the absence of reliable effective interactions, although the first feature supposedly can be treated with the aid of the exponential convergence method [91, 92] or similar approaches. The lack of knowledge of interactions requires more deep studies.

We have seen the possible vital role of the three-phonon couplings, as in eq. (51), in the development of enhancement. In the conventional RPA framework, such couplings are expressed by triangular diagrams, which come with a considerable reduction due to the combinations \(u_1u_2 - v_1v_2\) of the pairing coherence factors. This combination is antisymmetric with respect to the single-particle occupancies and would vanish in the case of full symmetry around the Fermi surface. This can be understood in analogy with the well known Furry theorem of quantum electrodynamics. In QED, such three-photon diagrams vanish exactly because of the precise cancellation of electron and positron contributions to the loop with three photon tails. In the discrete nuclear spectrum, there is no full symmetry and the result does not vanish but still it is considerably suppressed. Some systematic features of interplay between quadrupole and octupole degrees of freedom, as for example found in Refs. [76, 86], indicate that the three-phonon vertices should be stronger that it comes from the
RPA estimates.

This fact may have something to do with the effects of three-body forces whose role in many-body dynamics essentially is unknown. At this point it makes no difference what is the source of these forces; they can come from bare nucleon interactions\cite{93} or effectively result from the medium modifications. In the search for three-body interactions in heavy nuclei it would be natural to start looking for their collective effects\cite{94}. Such effects of cubic anharmonicity should be visible also in shape phase transitions in heavy nuclei. Indeed, the cubic quadrupole term in the collective potential energy, $\sim \beta^3 \cos(3\gamma)$ is responsible for sharp restructuring of single-particle orbitals and transition from gamma-unstable configurations typical for soft vibrators to the well deformed rotors. This topic definitely deserves further development.

VII. CONCLUSION

In this short review we tried to demonstrate the abundance of ideas and physical images related to the search of the effects of $\mathcal{P}, \mathcal{T}$-violating forces in atomic nuclei. Of course, there is immediate interest in measuring such effects which would lead us beyond the Standard Model, while currently we know only the upper limits. Because of extreme difficulty of such experiments and their time-consuming nature, it is important to try to establish the most promising path and to select nuclei where we can expect the most pronounced effects.

Along with that, it turns out that the wealth of physics related to the violation of fundamental symmetries in nuclei elucidates also many particular problems of nuclear structure which until now did not have definite answers. These problems are related to various manifestations of quantum-mechanical symmetries in a strongly interacting self-bound many-body system, such as the complex nucleus. Another open question is that of strong interaction between various collective and single-particle degrees of freedom.

Parity violation is known to be enhanced by the orders of magnitude by statistical (chaotic) properties of compound state neutron resonances. In the search for the $\mathcal{P}, \mathcal{T}$-violation we are looking for coherent effects. The EDM of the atoms is induced by the nuclear Schiff moment through its $\mathcal{P}, \mathcal{T}$-violating potential. The best perspectives for a significant enhancement of the nuclear Schiff moment are currently seen in the nuclei with static octupole deformation in the ground state. We argued that the soft octupole mode in
a combination with well developed quadrupole deformation is expected to display enhancement as well. Finally, we came to soft nuclei with slow quadrupole and octupole motion of large amplitude. Although the direct attempt in this direction did not yet bring desired results, we need to better understand nuclear physics of such nuclei where the shape is in fact ill-defined and the routine theoretical methods, such as the RPA, are probably not sufficient. This leads to new problems of structure of mesoscopic systems on the verge of shape instability. Another interesting question is that of the three-body residual forces (coming from bare three-body forces or induced by the nucleon correlations). Such forces may give stronger mode-mode coupling not limited by the Furry theorem discussed above. In general, the entire area of research is very promising for understanding the fundamental symmetries at work in a many-body environment.

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