Nuclei with enhanced Schiff moments in practical elements for atomic and molecular EDM measurements

This is a resource paper concerning enhancement of observable time-reversal breaking effects by nuclear structure, aimed at AMO experimentalists. It’s intended to support a white paper [1] by providing some orientation on what can be said about some particular isotopes. Any conclusions are qualitative, and the reader should consult and cite the primary references and reviews rather than this arXiv alone.

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1 Qualitative info on enhanced atomic and molecular EDM’s from nuclear phenomena

Many nuclei have low-lying excited states with same spin as the ground state and opposite parity. A number of these have recently been suggested in the AMO literature as possibly exhibiting static or vibrational octupole deformation. A goal is to identify practical candidates with enhanced Schiff moments in particular elements where advanced AMO techniques could offer increased sensitivity to boosted atomic and molecular EDM’s. Isotopes are sought in addition to $^{225}$Ra that are long-lived enough to use away from isotope production facilities [2, 3] or are producible from generators like $^{223}$FrAg [4, 5]. There is a similar need to choose quantifiably large Schiff moments in crystals with stable rare earth elements to optimize experiments searching for CP-violating couplings to long-wavelength axionlike dark matter [6]. Some of the new parity doublets suggested are supported by indirect experimental info, e.g. BE(3) strength measured or calculated in nearby even-even nuclei. Unfortunately, other nuclear structure phenomena that would not enhance Schiff moments can account for closely spaced parity doublets. Whether or not the ground state and higher-spin states built on it look like one of a pair of static or vibrational octupole bands, often there is limited information about the opposite-parity excited states. Considerable effort over three decades has gone into identifying definitive experimental nuclear signatures for static and vibrational octupole deformation for many nuclei [7, 8, 9, 10].

Here we examine informally to what extent a number of these suggested low-lying parity doublets would need more experimental nuclear structure information and/or microscopic calculations to identify and quantify possible Schiff moment enhancement. Whenever we list experimental evidence against static octupole deformation for a few interesting AMO cases, we try to qualify to what extent collective octupole vibrations can have similar Schiff moment enhancement.

Note that Ref. [1] considers AMO methods less element-specific, thus possibly applicable to any $Z \geq 86$ nucleus determined to have Schiff enhancements, including quantum logic spectroscopy [11], frozen noble gas hosts [12], and ultracold molecule clock states [13]. The possible parity doublet in $^{229}$Pa has energy splitting $60 \pm 50$ eV [14], and experiments to resolve its status are considered [15].

1This paper avoids the word ‘actinide,’ sensibly restricted to ‘f-element’ by AMO physicists— who spend years on their relatively complex atomic and molecular spectra– but used more broadly in the nuclear structure literature.
1.1 TRV enhancements from nuclear structure: background

A continuum between static octupole deformation and collective octupole vibrations. Schiff moment-induced atomic and molecular EDM’s are thought to be similar in systems with static octupole deformation and in systems with ‘soft’ (i.e. virtual) excitation of octupole vibrations that are more common, though those octupole vibrations must be collective to helpfully enhance the Schiff moment. Engel, Friar, and Hayes (EFH) \cite{EFH} discuss to what extent these extremes are different aspects of formally similar phenomena (see other reviews like Ref. \cite{Ref} for related discussions of octupole vibrations and static deformation), and showed that in macroscopic models a Schiff moment enhancement from collective octupole vibrations also scales with the inverse of the parity doublet’s energy splitting, with the static deformation $\langle \beta_3 \rangle^2$ replaced by the virtual deformation average $\langle \bar{\beta}_3 \rangle$. EFH point out additional physical effects that must be calculated for the vibrators, which could enhance the Schiff moment further. Flambaum and Zelovinsky apply a similar analytical calculation of collective octupole vibrations to cases of interest $^{223}$Rn and $^{223,225}$Ra, finding similar Schiff enhancement compared to previous calculations assuming static octupole deformation \cite{Flambaum}. Auerbach et al. \cite{Auerbach} with microscopic QRPA find similarly large Schiff moment enhancement from collective vibrations in the limit when their energies are small: they find in $Z \geq 86$ nuclei (with N and Z separated from the region of known static octupole deformation) that octupole vibrational configurations are only small components of the complex nuclear wavefunctions, suppressing the Schiff moment enhancement. Note that configurations are assumed purely octupole in some analytical approximation formulae, though Ref. \cite{Ref} calculates such a suppression factor. This author is unaware of any calculations that consider interference between static and collective vibrational effects, which presumably would be included naturally in future microscopic calculations \cite{Others}.

Nuclear magnetic quadrupole moments The possible enhancements of Schiff moments between two and five orders of magnitude from static octupole deformation have produced much attention in designing AMO experiments. Additionally, atomic and molecular EDM’s can be enhanced by other nuclear effects by about an order of magnitude, potentially leading to exciting discovery potential if the AMO experiment has sufficient sensitivity. Contributions of the more ubiquitous nuclear magnetic quadrupole moment (MQM) to atomic and molecular EDM’s are free from atomic shielding, so have been reliably calculated \cite{MQM}. MQM’s provide order-of-magnitude enhancement for any nucleus with quadrupole deformation and nuclear spin $\geq 1$, and if the atomic or molecular state has nonzero angular momentum. Experimental difficulties from the nonzero electron spin needed can be mitigated by choosing systems with small magnetic g-factor, allowing in principle long coherence times, and its known existence in many stable nuclei is driving dedicated experimental efforts \cite{MQM}. Experimental efforts are ongoing.

TRV matrix elements That all atomic EDM enhancements from nuclear structure also require difficult-to-calculate matrix elements of parameterized TRV hadronic interactions was made apparent in Ref. \cite{TRV}, with possible microscopic theoretical improvements of the spatial wavefunctions necessary highlighted in Ref. \cite{Others}. Some analytical formulae include an estimate of one TRV matrix element from a one-body effective potential \cite{Ref,Others}. There are no known helpful experimental benchmarks for the most important operator $\sigma \cdot p$ in heavy nuclei.
1.2 Observables

Only two observables are qualitatively discussed here—consult the reviews for complete information.

**Charge radii changes with neutrons** Adding a neutron to a nucleus increases its charge radius. For a given element, adding a neutron to an odd-N nucleus usually increases the charge radius by less than adding a neutron to an even-N nucleus—intuitively, this is reasonable when the extra neutron simply pairs in spin with the odd valence neutron in the same orbital, rather than populating another orbital or driving a change in collective properties. Octupole deformation is a possible explanation for unusual isotopes with inverted differences in neutron-induced change of charge radii (“IDNCR”) in Rn,Fr,Ra, with measurements further delineating IDNCR at higher neutron number and in Ac. Other explanations than octupole phenomena in lower-Z nuclei are considered in Ref. [30], which also mentions the possibility that collective vibrational effects might similarly produce IDNCR. For some isotopes, IDNCR is the only experimental information, yet thought it can be consistent with static octupole deformation or collective octupole vibrations, unfortunately can’t be definitive.

**BE(3)’s, BE(1)’s** A possible smoking gun is electric octupole transition strength B(E3) between the opposite-parity bands, but AMO people should recall the long-wavelength expansion works really well in nuclei \( r/\lambda \sim 1 \text{ MeV}/197 \text{ MeV}-\text{fm} \sim 0.5\% \). So if an E1 is allowed, the E3’s start smaller by over 8 orders of magnitude and are usually considered unmeasurable. Thus measurements of E3 strength between the ground 0\(^+\) state and excited 3\(^-\) state in nearby even-even nuclei are possible and useful. Strong B(E1)’s are expected between the opposite-parity bands of static octupole deformation, while weak B(E1)’s are often considered to be consistent with collective octupole vibrations: since there can be other reasons for either extreme, B(E1)’s are not considered definitive unless there are thorough theory considerations.

**Odd-odd nuclei** Note that nuclei with both odd N and odd Z can have octupole deformation, possibly doubling the number of cases with Schiff enhancement. However, the nuclear structure is so much more complicated than odd-even nuclei that it’s much less likely the Schiff enhancement could be definitively determined, either experimentally or theoretically.

2 Examples

Here are considerations of isotopes of AMO interest.

2.1 Rare earths

A number of rare earth elements have been laser-cooled and trapped, and several isotopes of such elements with low-lying parity doublets are being suggested for static octupole deformation. \(^{153}\)Eu has been examined thoroughly. \(^{152,154}\)Eu are odd Z-odd N nuclei with half-lives of 13 and 8 years that have structure and E1 strengths suggesting octupole deformation, while they and stable \(^{154}\)Eu exhibit IDNCR consistent with octupole deformation in the ground states. Such evidence inspired detailed experimental examination of excited states in \(^{153}\)Eu, and the g-factors of the identified excited opposite-parity band are known to be about 3 times larger than the ground state band. Now, it’s natural for perturbations such as Coriolis mixing to change properties of partner bands differently—nearby configurations tend to have the natural
parity of the ground-state—thus certain properties don’t have to be identical. Nevertheless, such
different g-factors discourage an interpretation of this doublet in $^{153}$Eu as exhibiting static octupole
deformation, while relatively large E1’s between the bands are hard to interpret in terms of octupole
vibrations $^{36}$ $^{37}$. So $^{153}$Eu remains ambiguous, and needs further modelling and calculation to
determine whether its identified parity doublet has octupole phenomena.

The case of $^{153}$Eu is apparently resolved: Sushkov, after pointing out the differing magnetic
moments of the $^{153}$Eu 5/2+ ground state and low-lying 5/2− state are inconsistent with the static
octupole model, calculates the admixture of octupole vibration to deformed Nilsson states, relating
the Schiff moment to experimental data on magnetic moments and E1 and E3 transition amplitudes
in odd-even nuclei and adjacent even-even nuclei. $^{153}$Eu is one of the few nuclei with all data needed,
and Ref. $^{38}$ finds 30x enhancement of the resulting Schiff moment of $^{153}$Eu over spherical nuclei
and estimates model uncertainty, finding a similar result for $^{237}$Np.

Other stable rare earths Several other stable rare earth isotopes have low-lying parity dou-
blets ($^{161,163}$Dy, $^{165}$Er, $^{155}$Gd, $^{153}$Sm) $^{2}$ $^{3}$, while nearby even-even nuclei with measured 3− states
and BE(3) strength support the possibility of collective vibrational octupole configurations in such
nuclei as well as in $^{155}$Eu $^{39}$. A recent global calculation of particle-bound even Z - even N nuclei
predicts static octupole deformation in the ground states of stable $^{146,148,150}$Nd and $^{150}$Sm $^{40}$,
while a region in Z and N of radioactive rare earth nuclei with much higher N than the line of
stability has been identified to have static octupole deformation, both experimentally and theoreti-
cally $^{40}$ $^{49}$ $^{33}$. These stable rare earth nuclei proposed for Schiff moment enhancements need
further experimental and/or microscopic theoretical supporting evidence for static or collective
vibrational octupole deformation in their ground and excited states.

2.2 $Z \geq 86$

AMO experiments have been considered for nuclei with supporting experimental evidence for static
octupole deformation and/or collective octupole vibrations for ground and excited states of a parity
doublet, including $^{225}$Ra, $^{223}$Fr, $^{225,227}$Ac, and $^{227,229}$Th (see Fig. 1).

Radium: The solid experimental evidence supporting static octupole deformation in I=1/2
$^{225}$Ra and I=3/2 $^{223}$Ra is thoroughly documented in review articles $^{9}$ $^{8}$.

Francium: $^{223}$Fr is an illustrative case where experiment and theory suggest a large enhance-
ment of the Schiff moment, even though the nuclear wavefunctions are thought to contain significant
admixtures of static octupole deformation and collective octupole vibrations. IDNCR exists for
$^{223,225}$Fr $^{29}$ $^{11}$ (it barely exists for $^{221}$Fr, a conclusion that does not change with a slightly revised
optical isotope shift $^{12}$). Concerning excited states, it’s instructive to note that $^{221}$Fr is a rather complex “transition” nucleus; e.g., its possible static octupole deformed excited parity-doublet
band actually has spins out of order in energy. This is understood as a case in neutron number N
between $^{219}$Fr, which has no special deformation, and $^{223}$Fr, which has “fairly strong” evidence $^{43}$
from its structure and feeding from alpha- and beta- decay for a static octupole deformation par-
ity doublet, albeit with a relatively large parity-doublet splitting of 161 keV. The experimental
parity doublet of $^{223}$Fr has been modelled including admixtures with static octupole and collective
coctupole vibrations $^{43}$; however, E1 transitions between the $^{223}$Fr bands were later found to be
relatively weak, consistent with $^{223}$Fr having collective octupole vibrations $^{44}$ $^{45}$ $^{46}$. Ref. $^{19}$,
which considers theoretical admixtures of other configurations in all its calculations, predicts the
Figure 1: Overly simplistic summary of $Z \geq 86$ isotopes of possible AMO interest that have experimental evidence suggesting extremes in the continuum of static octupole deformation vs. collective octupole vibrations, either of which can enhance TRV Schiff moments. Only the dominant configuration is indicated—see text and references for any details. Darker blues have longer half-lives (see ndc.bnl.gov).
static octupole enhancement of EDM’s for $^{221}$Fr to be an order of magnitude less than $^{223}$Fr and $^{225}$Ra. $^{225}$Fr has weak B(E1)’s inconsistent with static octupole deformation but consistent with collective octupole vibrations $^{46}$. (Note Ref. $^{46}$ has a thorough pedagogical discussion of the B(E1) phenomenology, including an updated figure of the B(E1)’s in Ref. $^{7}$.)

**Actinium:** $I^e=3/2$ $^{227}$Ac has a low-lying $3/2^+$ excited state, reviewed in $^{7}$. There is considerable evidence consistent with these being the lowest-lying states of bands with static octupole deformation, including measurements of g-factors. But there is also experimental evidence against static octupole deformation for this parity doublet, including measured BE(1)’s an order of magnitude smaller than other cases, and transfer reactions populating excited states that can be explained by reflection-symmetric potentials $^{7}$. $^{227}$Ac could be a case with large collective vibrational octupole enhancement, and EDM experiments involving actinium molecules $^{2}$ could also be done in $^{225}$Ac, which has strong supporting evidence for static octupole deformation $^{7}$ and a 10-day half-life producible by a $^{229}$Th generator.

**Thorium:** Some EDM experimental techniques work best for nuclear spin $I=1/2$. In addition to the well-known $I=1/2$ $^{225}$Ra, $^{227}$Th likely has $I=1/2$ $^{17}$. There is strong experimental and theoretical support for static octupole deformation with an identified parity double band for an $I=1/2$ ground state, and a large Schiff moment enhancement $^{8,9}$.

An explicit band of excited states is identified in $^{229}$Th as a vibrational octupole partner of a ground state band, with energy splitting 146 keV $^{48,49}$, and thus from the general expectations of Ref. $^{16}$ a full microscopic calculation could show a large Schiff moment for $^{229}$Th. It is in this sense that recent BE(1) measurements in $^{228}$Th supporting vibrational collective octupole effects in $^{229}$Th are considered to support it as an enhanced atomic or molecular EDM case $^{50}$, even though detailed consideration of the excited states of $^{229}$Th has classified it as a ‘transition’ isotope with larger $N$ than nuclei with demonstrated static octupole deformation $^{51,8}$.

**Radon:** IDNCR exists for $^{221,223}$Rn $^{25}$, but there is only one excited state energy known for $^{221}$Rn and no excited state info for $^{223}$Rn. Favorable static octupole arguments from early calculations $^{19}$ have been more recently weakened by BE(3) measurements in nearby even-even nuclei $^{9}$, which instead suggest collective vibrational octupole effects are possible $^{52}$. To quantify the Schiff enhancements would either way need detailed excited-state nuclear structure measurements, though this has remained elusive in several experimental attempts.

**Summary** All nuclei with reasonably definitive supporting experimental evidence for static octupole deformation are radioactive, with half-lives on the order of weeks or shorter. Longer-lived nuclei like $^{229}$Th and $^{227}$Ac, along with stable rare earth isotopes, show evidence for collective octupole vibrations that could also produce quantifiably large Schiff enhancements, if microscopic calculations with sufficiently small uncertainty can be developed. Any prospective parity doublet needs support from experimental observables to define what fraction of the ground state and excited states have static or collective vibrational octupole configurations. Microscopic theory improvements of this aspect, as well as to quantify matrix elements of the several TRV isospin- and range-dependent interactions $^{20}$, would enable a move from the current exciting discovery phase to defining multiple complementary experiments to extract different microscopic sources of TRV.

**Acknowledgements** P. Butler, J. Engel, N. Hutzler, A. Jayich, D. DeMille, A. Vutha, W. Nazarewicz, A. Madden, G. Neyens, and G. Hackman all have had helpful comments and/or orientation. The author notes that two nuclear theorists calculating Schiff moments share surnames with AMO experimentalists in this field—the AMO community should be inspired to encourage
any further relatives to help. This author is, of course, responsible for any misinterpretations of the literature.

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