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Time-reversal violation in heavy octupole-deformed nuclei

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Abstract. A nonzero atomic electric-dipole moment (EDM) at a level not far from current experimental limits would signify time-reversal violation from outside the Standard Model. EDMs are enhanced in atoms that have octupole-deformed nuclei. We report a careful self-consistent mean-field calculation of the time-reversal-violating nuclear Schiff moment —the quantity that induces an atomic EDM— in the octupole-deformed nucleus ^{225}Ra. The self-consistent mean field in odd-A nuclei includes important effects of core polarization. The results of the calculation are encouraging for EDM experiments in the light actinides. Accurate calculations of Schiff moments in ordinary spherical and quadrupole-deformed nuclei such as ^{199}Hg are also important. We describe work in progress on this more general problem.

PACS. 11.30.Er General theory of fields and particles: Charge conjugation, parity, time reversal, and other discrete symmetries – 21.60.Jz Nuclear structure: Hartree-Fock and random-phase approximations

1 Introduction

Experiments with kaons and B-mesons indicate that time-reversal invariance (T) is violated at a low level. The results of these experiments can be explained by a phase in the Cabibo-Kobayashi-Maskawa (CKM) matrix of the Standard Model. But the absence of antimatter in our universe is evidence that T invariance (or more precisely, CP invariance) was badly violated long ago. The CKM phase is unable to account for so large an effect, and so theorists believe there must be another source of T violation, this one from outside the Standard Model.

As we shall see, an atom in its ground state cannot have an electric dipole moment (EDM) without violating T. A number of experiments have searched for atomic EDMs, and the limits are tight. But because CKM T violation shows up in first order only in flavor-changing processes, it should appear in atomic experiments only after the limits are improved by 5 or 6 orders of magnitude. The same constraint does not apply, however, to T violation in extensions to the Standard-Model. The most popular extension, supersymmetry, has many flavor-conserving phases, making EDM experiments ideal for testing it. Already these experiments are putting serious pressure on the theory.

Here, after some preliminaries, we argue that experiments on atoms with octupole-deformed nuclei will be more sensitive to T-violation within the nucleus than the current best experiments. The enhancement of T violation in these nuclei is connected with the collective violation of intrinsic parity. This paper discusses work published by the author together with Jim Friar and Anna Hayes [1] and Michael Bender, Jacek Dobacewski, Joao de Jesus, and Piotr Olbratowski [2], and some work in progress on spherical nuclei with Joao de Jesus.

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2 T violation and EDMs

2.1 Why do EDMs require T violation?

It is obvious that for the negative-parity (P) dipole operator to have a non-zero expectation value in a non-degenerate state, P must be violated. But because states with good J, M are not eigenstates of the T operator, the usual argument from "good quantum numbers" does not work for T. Why must it be violated as well?

Consider a state $|g; J, M\rangle$ (g stands for "ground") with no degeneracy besides the $2J+1$ spin multiplicity. Symmetry under rotation by π around the y axis implies that for a vector operator such as $\boldsymbol{d} \equiv \Sigma_i e_i \boldsymbol{r}_i$,

$$\langle g: J, M|\boldsymbol{d}|g: J, M\rangle = -\langle g: J, -M|\boldsymbol{d}|g: J, -M\rangle. \quad (1)$$

The time reversal operator $\hat{T}$ takes $|g: J, M\rangle$ to a real phase times $|g: J, -M\rangle$ (under the usual phase conventions), just like rotation by π. But $\boldsymbol{d}$ does not change under $\hat{T}$, while the rotation flips its sign. So if the system is invariant under T, we also have

$$\langle g: J, M|\boldsymbol{d}|g: J, M\rangle = +\langle g: J, -M|\boldsymbol{d}|g: J, -M\rangle. \quad (2)$$

These two equations together imply that $\langle \boldsymbol{d} \rangle$ must vanish. If T is *violated*, the argument fails because $\hat{T}$ will take

$|g : J, -M\rangle$ to a state with J, $-M$ that is not identical to the corresponding member of the ground-state multiplet. In that case, eq. (2) does not hold.

2.2 How objects get EDMs and why atomic EDMs are suppressed

T-violation can work its way up from the most fundamental particles through to atoms. If the symmetry is violated by, *e.g.* supersymmetry, quarks will develop T-violating couplings, leading to effective T-violating πNN couplings. These in turn lead through pion exchange to an effective two-nucleon interaction of the form

$$\begin{aligned} H_T = -\frac{g\, m_\pi^2}{8\pi m_N} \Big\{ &(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \cdot (\boldsymbol{r}_1 - \boldsymbol{r}_2) \Big[\bar{g}_0\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ &- \frac{\bar{g}_1}{2} (\tau_{1z} + \tau_{2z}) + \bar{g}_2 (3\tau_{1z}\tau_{2z} - \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \Big] \\ &- \frac{\bar{g}_1}{2} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\boldsymbol{r}_1 - \boldsymbol{r}_2) (\tau_{1z} - \tau_{2z}) \Big\} \\ &\times \frac{\exp(-m_\pi |\boldsymbol{r}_1 - \boldsymbol{r}_2|)}{m_\pi |\boldsymbol{r}_1 - \boldsymbol{r}_2|^2} \left[1 + \frac{1}{m_\pi |\boldsymbol{r}_1 - \boldsymbol{r}_2|} \right], \end{aligned} \tag{3}$$

where g is the normal strong πNN coupling constant and the three $\bar{g}$'s are dimensionless isoscalar, isovector, and isotensor T-violating πNN couplings. This interaction can cause the nucleus to develop an EDM, which in turn causes an atomic EDM. The goal of the atomic experiments (and this work) is to extract limits on the $\bar{g}$'s from experimental limits on an atomic EDM, or to determine them if an EDM is observed.

Unfortunately, atomic EDMs are suppressed. Any nuclear EDM induced by the interaction in eq. (3) is shielded by the electrons, which rearrange themselves to create an electronic EDM in the opposite direction. Schiff proved [3] that the cancellation is exact in the limit of a point-like nucleus and nonrelativistic electrons[1].

Luckily, the nucleus has a finite radius so the shielding is not complete. It turns out, however, that after its effects are accounted for, the nuclear quantity that induces an EDM in the electrons is not the dipole moment $\boldsymbol{D}$, but rather a kind of weighted dipole moment (with a correction term) called the "Schiff moment":

$$\boldsymbol{S} = \frac{1}{10} \sum_p e_p \left[r_p^2 - \frac{5}{3} R^2 \right] \boldsymbol{r}_p\,, \tag{4}$$

where R^2 is the root-mean-squared nuclear charge-density radius. If, as one would expect, $\langle \boldsymbol{S} \rangle \approx 0.1 R^2 \langle \boldsymbol{D} \rangle$, then the atomic EDM $\boldsymbol{d}$ is down from $\langle \boldsymbol{D} \rangle$ by $O(R^2/10R_A^2) \approx 10^{-9}$. ($R_A$ is the atomic radius.) But the behavior of relativistic Coulomb wave functions near the origin partly offsets this terrible suppression via a factor $10Z^2 \approx 10^5$ in heavy nuclei, so that the overall suppression of the atomic EDM from shielding is only about 10^{-4}. This number begins to approach the factor by which EDM limits on the neutron are worse than atomic limits, and the nuclear Schiff moment is more sensitive to neutral pion exchange than the neutron EDM, so atomic experiments are currently competitive in the search for some kinds of T violation.

[1] It may be possible to reduce or eliminate shielding in experiments with "naked nuclei" [4,5].

3 Enhancement by octupole deformation

We can make atomic experiments even more attractive by finding the right atom, because some atoms are better places to look for an EDM than others. One reason is that octupole deformation of atomic nuclei enhances the nuclear Schiff moment dramatically.

Since the T-violating interaction H_T is very weak, it can be treated peturbatively, and the Schiff moment can be written as

$$\langle \boldsymbol{S} \rangle = \sum_m \frac{\langle 0|\boldsymbol{S}|m\rangle \langle m|H_T|0\rangle}{E_0 - E_m} + \text{c.c.} \tag{5}$$

Two collective effects associated with octupole deformation make this expression large. The first is the existence of parity doubling. The intrinsic state has a shape that breaks parity symmetry. It contains both positive- and negative-parity components, and when projected onto good parity yields two states of opposite parity very close to one another in energy. In ^{225}Ra, for example, the $J^\pi = 1/2^+$ ground state ($|0\rangle$ in our notation) has a $J^\pi = 1/2^-$ partner $|\bar{0}\rangle$ just 55 keV higher. Since H_T is pseudoscalar, it connects $|0\rangle$ and $|\bar{0}\rangle$, and the single term with $|\bar{0}\rangle$ as the intermediate state dominates the sum in eq. (5). Just like for quadrupole transitions, the transition matrix element $\langle 0|\boldsymbol{S}|\bar{0}\rangle$ is proportional to the intrinsic Schiff moment, so that eq. (5) becomes, to good approximation,

$$\langle \boldsymbol{S} \rangle \approx -2/3 \frac{\langle \boldsymbol{S}^{\text{intr.}} \rangle \langle H_T \rangle}{E_0 - E_{\bar{0}}}\,. \tag{6}$$

The second collective enhancement comes from robust intrinsic Schiff moments that often are much larger than R^2 times the intrinsic dipole moment. Although the intrinsic dipole moments in octupole-deformed nuclei are collective, they are often quite small. The reason is that they depend on the distribution of charge *with respect to the center of mass*, and vanish when the neutron and proton densities coincide exactly. Intrinsic Schiff moments are not subject to this kind of cancellation. As a result of this and the parity-doubling, the laboratory Schiff moment in a nucleus like ^{225}Ra is enhanced, according to collective model estimates [6,7] by two or three orders of magnitude over that of ^{199}Hg, the atom with the best experimental limit on its EDM [8].

Why is the uncertainty an order of magnitude, a factor large enough to deter experimentalists? The matrix element of H_T depends on the nuclear spin distribution, a delicate quantity. In simple collective models (such as the particle-rotor model) a single valence nucleon carries all the spin. In reality, however, the valence nucleon polarizes the core, an effect that can alter the spin distribution

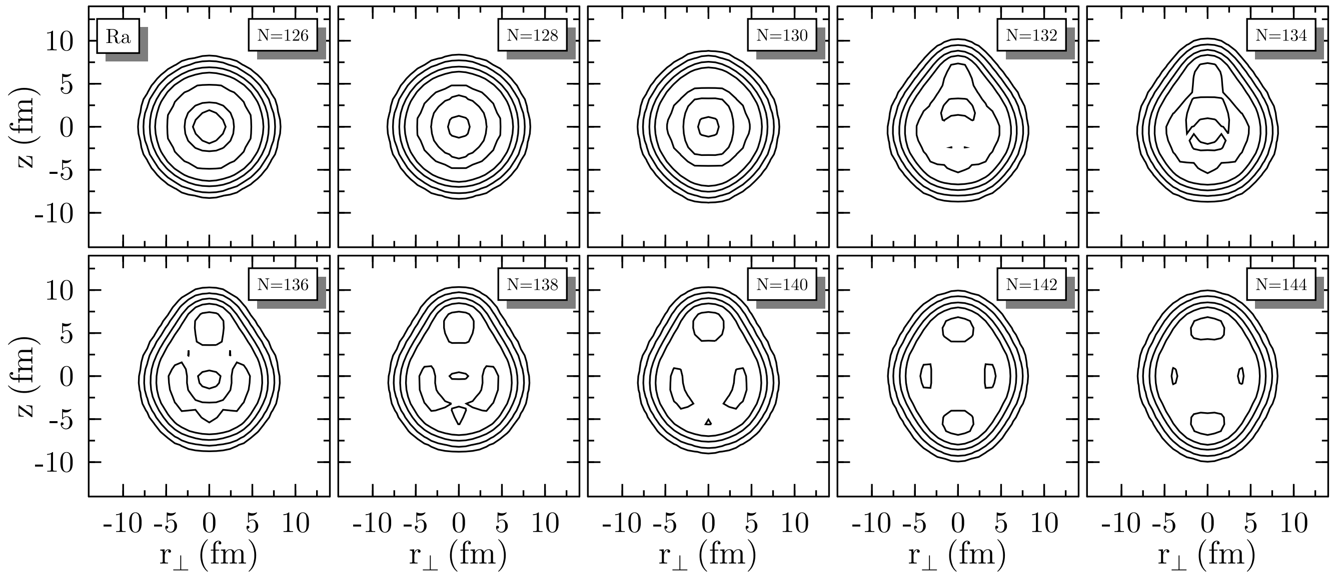

Fig. 1. Contours of constant density for a series of even-N radium isotopes. Contour lines are drawn for densities $\rho = 0.01$, $0.03, 0.07, 0.11$, and $0.15\,\mathrm{fm}^{-3}$.

substantially. Even without core polarization, the matrix element of H_T depends sensitively on the wave function of the valence nucleon. To reduce the uncertainty in the Schiff moment to a reasonable level, we need a state-of-the art calculation.

4 Calculation of Schiff moment in ^{225}Ra

In ref. [2] we used the program HFODD [9] to do a completely self-consistent Skyrme-mean-field calculation of the intrinsic ground state of ^{225}Ra. The code allows the simultaneous breaking of rotational invariance, P, and T. The first two are needed to obtain octupole deformation, the last to polarize the core (*i.e.* break Kramers degeneracy). HFODD cannot yet treat pairing when it allows T to be broken, but pairing in T-odd channels is poorly understood. No no existing codes can do more than HFODD in odd-A octupole-deformed nuclei.

We used the Skyrme interactions SIII, SkM*, SLy4, and SkO$'$, the last our favorite because it was tuned in ref. [10] to treat spin degrees of freedom (particularly isovector spin excitations). Figure 1 shows the shapes produced by SkO$'$ in the even Ra isotopes. The nucleus ^{225}Ra, with $N = 137$, will clearly have significant amounts of both quadrupole and octupole deformation.

Figure 2 shows three parity-violating intrinsic quantities. In the top panel is the ground-state octupole deformation as a function of neutron number. The trend mirrors that in the density profiles shown earlier. The second panel shows the absolute values of intrinsic dipole moments D_0, along with experimental data extracted from $E1$ transition probabilities [11]. Both the experimental and calculated values change sign between $N = 134$ and $N = 138$, illustrating the delicacy of this quantity. None of the forces precisely reproduces the trend through all the isotopes,

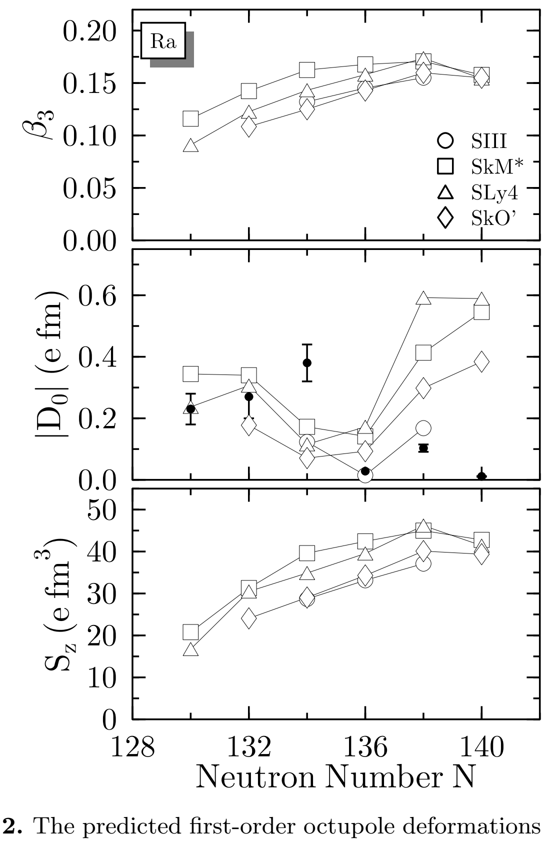

Fig. 2. The predicted first-order octupole deformations (top), absolute values of the predicted intrinsic dipole moments (middle), and the predicted intrinsic Schiff moments (bottom) for four Skyrme interactions in a series of even-N radium isotopes. The absolute values of the experimental intrinsic dipole moments are also shown.

but the comparison has to be taken with a grain of salt because "data" derive from transitions between excited rotational states. The intrinsic Schiff moment $\langle S_z \rangle$, as noted

Table 1. Intrinsic-state expectation values of important operators in U_T, in the neutron-proton scheme (in $10^{-3}\,\mathrm{fm}^{-4}$).

	$\langle \boldsymbol{\sigma}_n \cdot \boldsymbol{\nabla}\rho_n \rangle$	$\langle \boldsymbol{\sigma}_n \cdot \boldsymbol{\nabla}\rho_p \rangle$
SIII(0)	−0.577	−0.491
SkM*(0)	−0.619	−0.120
SLy4(0)	−0.628	−0.050
SkO′(0)	−0.331	−0.013
SkO′	−0.320	−0.114
particle-rotor [7]	−1.2	−0.8

above, is more collective and under better control, as the bottom panel of the figure shows.

Finally, what about H_T? In the limit of infinite pion mass, eq. (3) reduces to an effective one-body potential

$$\hat{U}_T(\boldsymbol{r}) = -\frac{g}{2m_\pi^2 m_N}\sum_{i=1}^{A} \boldsymbol{\sigma}_i \tau_{z,i} \cdot \left[(\bar{g}_0+2\bar{g}_2)\boldsymbol{\nabla}\rho_1(\boldsymbol{r}) - \bar{g}_1\boldsymbol{\nabla}\rho_0(\boldsymbol{r})\right] + \text{exchange}, \quad (7)$$

where ρ_0 and ρ_1 are the isoscalar and isovector densities and exchange terms are probably negligible. Table 1 shows matrix elements of the most important operators in U_T.

The zeros following the interaction names mean that the core-polarizing parts of the interactions, which were never fit for the older forces, have been turned off. The differences between the lines labeled SkO′(0) and SkO′ show the effects of core polarization. Our full SkO′ Schiff moment for ^{225}Ra, with the finite-range force (though not yet with exchange terms or short-range correlations), is

$$\langle S_z \rangle_{\mathrm{Ra}} = -1.90\, g\bar{g}_0 + 6.31 g\bar{g}_1 - 3.80\, g\bar{g}_2 \;(e\,\mathrm{fm}^3). \quad (8)$$

A recent calculation for ^{199}Hg [12] gave

$$\langle S_z \rangle_{\mathrm{Hg}} = 0.0004\, g\bar{g}_0 + 0.055\, g\bar{g}_1 + 0.009\, g\bar{g}_2 \;(e\,\mathrm{fm}^3). \quad (9)$$

Our Schiff moment, though smaller than particle-rotor estimates, is over 100 times larger (and significantly more than that if $\bar{g}_1$ is anomalously small) than that of ^{199}Hg. Combined with an additional factor-of-three enhancement from atomic physics [13], this result bodes well for upcoming experiments [14] to measure the EDM of ^{225}Ra.

5 Schiff moment of ^{199}Hg

To be sure of the enhancement factor, and to discern the consequences of existing EDM limits, we need to be more confident of the Schiff moment of ^{199}Hg. Reference [12] predicts a very weak sensitivity to the isoscalar πNN coupling $\bar{g}_0$ (the first coefficient in eq. (9)). J. de Jesus and the author are calculating the Hg Schiff moment with the same Skyrme interactions we used in Ra. Our approach is to treat ^{198}Hg as a spherical core in the HFB approximation, and then include polarizing effects of the extra neutron quasiparticle in perturbation theory by allowing it to excite core vibrations, which we treat in QRPA. Figure 3

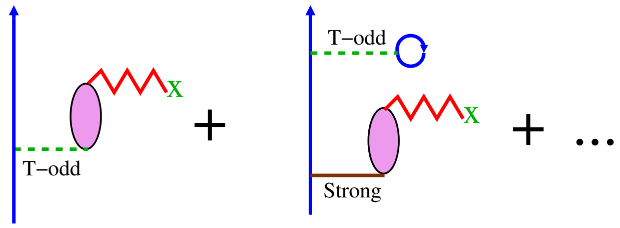

Fig. 3. Leading contributions to the Schiff moment of ^{199}Hg. The vertical line is the valence neutron, the solid horizontal line a Skyrme interaction, the dashed line H_T, the zig-zag line the Schiff operator, and the filled oval an RPA bubble sum.

shows the leading diagrams in the approximation that pairing effects are negligible (we include pairing in the actual calculations). The physics is similar to that included in ref. [12], but our calculation is more self-consistent and our use of several Skyrme interactions gives us a handle on the uncertainty. Our preliminary (still unofficial) result with SkO′ is

$$\langle S_z \rangle_{\mathrm{Hg}}^{\mathrm{prelim.}} = 0.007\, g\bar{g}_0 + 0.067\, g\bar{g}_1 + 0.009\, g\bar{g}_2 \;(e\,\mathrm{fm}^3), \quad (10)$$

and each of the coefficients changes by factors of 2 or 3 when we change the Skyrme interaction. Our isoscalar coefficient is considerably larger than the one in eq. (9). We will remove the tag "preliminary" as soon as we have explored the uncertainty a little more carefully.

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