Nuclear Time-Reversal Violation and the Schiff Moment of ^{225}Ra

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We present a comprehensive mean-field calculation of the Schiff moment of the nucleus ^{225}Ra, the quantity that determines the static electric-dipole moment of the corresponding atom if time-reversal (T) invariance is violated in the nucleus. The calculation breaks all possible intrinsic symmetries of the nuclear mean field and includes, in particular, both exchange and direct terms from the full finite-range T-violating nucleon-nucleon interaction, and the effects of short-range correlations. The resulting Schiff moment, which depends on three unknown T-violating pion-nucleon coupling constants, is much larger than in ^{199}Hg, the isotope with the best current experimental limit on its atomic electric-dipole moment.

The standard model of particle physics violates time-reversal (T) invariance, but apparently only through a single phase in the Cabibbo-Kobayashi-Maskawa matrix that mixes quark flavors. The resulting T violation in flavor-conserving observables is therefore very weak, and static electric-dipole moments (EDMs) of neutrons, electrons, or atoms, all of which are nonzero if T is violated, have never been observed. Standard-model T violation is also too weak to account for the baryon asymmetry of the universe, which must come from as yet undiscovered physics. Happily, most theories of what lies beyond the standard model contain enough phases that flavor-conserving T violation will be unsuppressed. Current levels of sensitivity in EDM experiments are already sufficient to rule out or pressure many extrastandard models, and it seems quite possible that with slightly improved sensitivity, new T-violating physics will be discovered.

Some of the tightest constraints on T violation come from atomic EDM experiments. The best of these at present is an experiment [1] with ^{199}Hg, but it has become clear recently [2–4] that atoms with octupole-deformed nuclei are potentially more sensitive than Hg. The primary reason is that given any T violation in the nucleon-nucleon interaction, an asymmetric nuclear shape and an associated parity doubling create a collective nuclear "Schiff" moment, a kind of radially weighted dipole moment (see below). (Earlier papers on T violation in polar diatomic molecules [5] and parity violation in fission [6] were the first to consider the effects of asymmetric shapes on fundamental symmetries. Reference [7] drew early attention to the importance for EDMs of low-lying nuclear states with the same angular momentum as the ground state but opposite parity.) Because of screening by atomic electrons, the Schiff moment, rather than the nuclear EDM, is the quantity that directly induces an atomic EDM (at least in

lowest order; see Ref. [8]). In nuclei with symmetric shapes, a collective contribution to the Schiff moment develops only in fluctuations around that shape [4,9].

In this Letter we calculate the Schiff moment of ^{225}Ra, or more precisely its dependence on any T-violating πNN couplings, in a mean-field theory that allows us to break all possible symmetries, consider a variety of phenomenologically successful strong (Skyrme) interactions, implicitly include the RPA polarization of the even-even core by the valence neutron, treat both the direct and exchange parts of the full pion-mediated interaction responsible for creating the Schiff moment, and include short-range two-body correlations between nucleons that modify the effects of this T-violating interaction. Though further refinements are possible, they will probably have to include correlations beyond mean-field theory and/or careful and systematic work on Skyrme functionals; the results presented here will not be easy to supersede.

Simpler calculations of Schiff moments have been attempted before. Reference [10] applied an independent-particle model in ^{199}Hg, ^{129}Xe, and other symmetrically deformed or spherical isotopes. References [11,12] carried out a much more sophisticated RPA-based calculation in ^{199}Hg; its main drawback was the use of a single phenomenological interaction that made it difficult to estimate uncertainty. Reference [3] made estimates in a particle-rotor model of the enhancement due to octupole deformation, and in Ref. [13], together with Bender, de Jesus, and Olbratowski, we applied a preliminary version of our technique to ^{225}Ra, an experiment on which is in the works [14]. That paper, however, assumed the range of the T-violating interaction to be zero, an especially bad approximation for exchange matrix elements, and was unable (obviously) to examine the effects of short-range NN correlations.

We briefly review some definitions and ideas. The Schiff moment is given accurately by the first-order expression

$$S \equiv \langle \Psi_0 | \hat{S}_z | \Psi_0 \rangle = \sum_{i \neq 0} \frac{\langle \Psi_0 | \hat{S}_z | \Psi_i \rangle \langle \Psi_i | \hat{V}_{PT} | \Psi_0 \rangle}{E_0 - E_i} + \text{c.c.}, \quad (1)$$

where $|\Psi_0\rangle$ is the member of the ground-state multiplet with $J_z = J = 1/2$ (positive parity), the sum is over ex-

cited states, and $\hat{S}_z$ is the operator

$$\hat{S}_z = \frac{e}{10} \sum_p \left(r_p^2 - \frac{5}{3} \bar{r}_{\text{ch}}^2 \right) z_p, \quad (2)$$

with the sum here over protons, and $\bar{r}_{\text{ch}}^2$ the mean-square charge radius. The operator $\hat{V}_{PT}$ in Eq. (1) is the T- (and parity-) violating nucleon-nucleon interaction mediated by the pion [7,15]:

$$\hat{V}_{PT}(\mathbf{r}_1 - \mathbf{r}_2) = -\frac{gm_\pi^2}{8\pi m_N} \left\{ (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \cdot (\mathbf{r}_1 - \mathbf{r}_2) \left[\bar{g}_0 \vec{\tau}_1 \cdot \vec{\tau}_2 - \frac{\bar{g}_1}{2}(\tau_{1z} + \tau_{2z}) + \bar{g}_2(3\tau_{1z}\tau_{2z} - \vec{\tau}_1 \cdot \vec{\tau}_2) \right] \right.$$

$$\left. - \frac{\bar{g}_1}{2}(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{r}_1 - \mathbf{r}_2)(\tau_{1z} - \tau_{2z}) \right\} \frac{\exp(-m_\pi|\mathbf{r}_1 - \mathbf{r}_2|)}{m_\pi|\mathbf{r}_1 - \mathbf{r}_2|^2} \left[1 + \frac{1}{m_\pi|\mathbf{r}_1 - \mathbf{r}_2|} \right], \quad (3)$$

where arrows denote isovector operators, τ_z is $+1$ for neutrons, m_N is the nucleon mass, and (in this equation only) we use the convention $\hbar = c = 1$. The $\bar{g}$'s are the unknown isoscalar, isovector, and isotensor T-violating pion-nucleon coupling constants, and g is the usual strong πNN coupling constant.

The asymmetric shape of ^{225}Ra implies parity doubling (see, e.g., Ref. [16]), i.e., the existence of a very low-energy $|1/2^-\rangle$ state, in this case 55 keV [17] above the ground state $|\Psi_0\rangle \equiv |1/2^+\rangle$, that dominates the sum in Eq. (1) because of the corresponding small denominator. With the approximation that the shape deformation is rigid, the ground state and its negative-parity partner in the octupole-deformed nucleus are projections onto good parity and angular momentum of the same "intrinsic state" (see Fig. 1), which represents the wave function of the nucleus in its own body-fixed frame with the total angular momentum aligned along the symmetry axis. Equation (1) then reduces to [3]
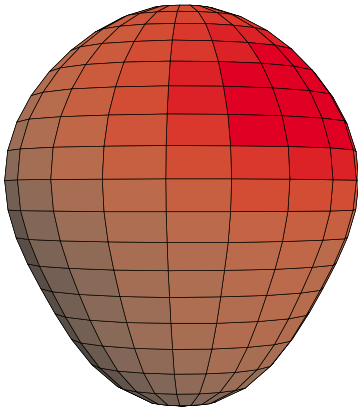

FIG. 1 (color online).   Shape of the microscopically calculated [13] mass distribution in ^{225}Ra, represented here by the surface of a uniform body that has the same multipole moments $Q_{\lambda 0}$ for $\lambda = 0, \ldots, 4$ as our calculated density.

$$S \approx -\frac{2}{3} \langle \hat{S}_z \rangle \frac{\langle \hat{V}_{PT} \rangle}{(55 \text{ keV})}, \quad (4)$$

where the brackets indicate expectation values in the intrinsic state. Using Eq. (3) for $\hat{V}_{PT}$, we can express the dependence of the Schiff moment on the undetermined T-violating πNN vertices as

$$S = a_0 g \bar{g}_0 + a_1 g \bar{g}_1 + a_2 g \bar{g}_2. \quad (5)$$

The coefficients a_i, which are the result of the calculation, have units $e \, \text{fm}^3$.

The octupole deformation enhances $\langle \hat{S}_z \rangle$, the first factor in Eq. (4), making it collective, robust, and straightforward to calculate with an error of a factor of 2 or less. The interaction expectation value $\langle \hat{V}_{PT} \rangle$ is harder to estimate because it is sensitive to the nuclear spin distribution, which depends on delicate correlations near the Fermi surface. Our calculation allows the breaking of Kramers degeneracy in the intrinsic frame and, consequently, spin polarization.

To evaluate $\langle \hat{V}_{PT} \rangle$ we constructed a new version of the code HFODD (v2.14 e) [18,19]. The code uses a triaxial harmonic-oscillator basis and Gaussian integration to solve self-consistent mean-field equations for zero-range Skyrme interactions. Evaluating matrix elements of the finite-range interaction (3) is much harder numerically, but efficient techniques have already been developed [20] for Gaussian interactions, which are separable in three Cartesian directions. The spatial dependence in Eq. (3) is different, the derivative of a Yukawa function, and we also include short-range correlations between nucleons (which the mean field does not capture) by multiplying the interaction by the square of a correlation function [21] that cuts off the two-nucleon wave functions below a relative distance of about a Fermi:

$$f(r) = 1 - e^{-1.1r^2}(1 - 0.68r^2), \quad (6)$$

with $r \equiv |\mathbf{r}_1 - \mathbf{r}_2|$ in Fermis and the coefficients of r^2 in

fm^{-2}. The resulting product looks very different from a Gaussian, but we were able to reproduce it quite accurately (see Fig. 2) with the sum of four Gaussians:

$$g(r) \equiv f(r)^2 \frac{e^{-a_\pi r}}{r^2}\left(1 + \frac{1}{a_\pi r}\right)$$

$$\approx 1.75e^{-1.1r^2} + 0.53e^{-0.68r^2} + 0.11e^{-0.21r^2}$$

$$+ 0.004e^{-0.06r^2}, \qquad (7)$$

where $a_\pi \equiv 0.7045$ fm^{-1} is the pion mass in inverse Fermis and the numbers in the fit all have units fm^{-2}. The extra factor of r not included in Eq. (7) [i.e., the factor $r_1 - r_2$ in Eq. (3)] is treated separately.

HFODD works with any Skyrme energy functional. In the context of the present study the best is SkO′ [22,23]. The "time-even" terms in this interaction, which act in even-nucleus ground states, were fit with special attention to nuclei around ^{208}Pb and to spin-orbit splitting. The "time-odd" terms responsible for core polarization in an odd nucleus were adjusted in Ref. [23] to reproduce Gamow-Teller resonances, resulting in an effective Landau parameter $g_0' = 1.2$. (The isoscalar parameter was set to $g_0 = 0.4$, following common practice.) For comparison, we also carry out the calculation with the older parametrizations SIII, SkM*, and SLy4 (with time-odd terms that are not fixed by gauge invariance neglected, and then again, with the simplest time-odd terms modified so that the Landau parameters have the same values as in SkO′) but have the most confidence in SkO′. Reference [13] presented predictions by these functionals for the binding energies, separation energies, intrinsic dipole moments, and spin-orbit splittings in the even Ra isotopes. SkO′ and SIII seemed to do the best job.
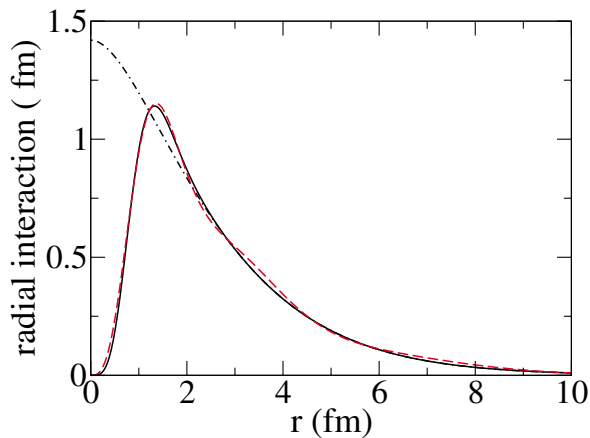

FIG. 2 (color online). The function $g(r)$ in Eq. (7) multiplied by r^3 (solid line), the Gaussian fit multiplied by r^3 (dashed line), and $r^3 g(r)/f(r)^2$, the radial T-odd interaction without short-range correlations (dot-dashed line). The factor r^3 is to account for the volume element and the additional factor of $r \equiv r_1 - r_2$ in Eq. (3).

Table I shows the calculated values, with SkO′, of the three coefficients a_i at several levels of approximation. The finite range reduces the direct matrix elements of the interaction (and the corresponding a_i) from the zero-range limit [13] significantly. The exchange terms are reduced much more, so that they are always smaller than the direct terms. The effects of the short-range correlations, which also reduce the coefficients, are relatively small as well but non-negligible. Finally, as pointed out in Ref. [8], relativistic effects in electron wave functions correct the effects of the Schiff moment; the authors summarize the corrections in a quantity they call the "local nuclear dipole moment." Our local dipole moment in ^{225}Ra is 82% of the Schiff moment for the $s_{1/2}$-$p_{1/2}$ atomic transition and 87% for the $s_{1/2}$-$p_{3/2}$ transition.

The coefficients produced by the forces we favor less, with the time-odd terms adjusted as mentioned above, are presented in Table II; SIII produces numbers similar to those of SkO′, while the other two forces give numbers that are larger by factors of 2 or 3, whether or not the Landau parameters are adjusted (i.e., the effects of adjusting those parameters seem to be fairly small).

What is the uncertainty in our numbers? The mean field omits correlations that could have some effect on the result; those could be explored by refining the calculation through angular momentum and parity projection, i.e., the restoration of symmetries broken by the mean field. In addition, an optimal Skyrme functional has yet to be identified. Those we tested give results that differ from the SkO′ numbers by factors of 2 or 3, as mentioned above. But some low-order terms in the T-odd part of the Skyrme functional are never used even in SkO′, because they have never been fit. Reference [23] constrained some combinations of those terms, but others were set to zero for lack of sufficient Gamow-Teller data in spherical nuclei. One might imagine trying to fit in deformed nuclei, or looking at spin-strength distributions with different total angular momentum and parity; the 0^- channel would be particularly useful because those are the quantum numbers of $\hat{V}_{PT}$. At the same time, it would probably help to explicitly study the sensitivity of the Schiff moments to changes in the various Skyrme parameters, both in the time-odd and time-even sectors. With enough work on all these fronts, we

TABLE I. Coefficients of $g\bar{g}_i$, in units of e fm^3, in the expression Eq. (5) for the Schiff moment of ^{225}Ra, calculated with the SkO′ Skyrme interaction. The abbreviation "src" stands for "short-range correlations."

	a_0	a_1	a_2
Zero range (direct only)	−5.1	10.4	−10.1
Finite range (direct only)	−1.9	6.3	−3.8
Finite range + src (direct only)	−1.7	6.0	−3.5
Finite range + src (direct+exchange)	−1.5	6.0	−4.0

TABLE II. Same as the last line in Table I but for the SIII, SkM*, and SLy4 interactions.

	a_0	a_1	a_2
SIII	-1.0	7.0	-3.9
SkM*	-4.7	21.5	-11.0
SLy4	-3.0	16.9	-8.8

could give a firmer estimate of the uncertainty than our current guess: a factor of 2 or 3.

If we accept our current results as reasonably accurate, we are in a position to quantify the advantages of ^{225}Ra for an EDM measurement. The recent RPA calculation [11,12] of the a_i for ^{199}Hg gives

$$^{199}\text{Hg}: \quad a_0 = 0.0004, \qquad a_1 = 0.055, \qquad a_2 = 0.009. \tag{8}$$

Our numbers are more than 2 orders of magnitude larger, particularly in the isoscalar channel (the relevant channel if T violation is caused by a nonzero QCD parameter $\bar{\theta}$), where the Hg number is anomalously small. Atomic physics enhances any EDM in Ra by another factor of 3 over that in Hg [24], so if the Ra EDM can be measured even $1/100$th as accurately as that of Hg, the sensitivity to nuclear T violation will be significantly greater.

In conclusion, we have evaluated the Schiff moment of ^{225}Ra in a completely symmetry-breaking mean-field approach, including, in particular, the finite-range matrix elements of the T violating nucleon-nucleon interaction. The results indicate that EDM experiments in this system are very promising. The remaining uncertainty of a factor of 2 or 3 is related primarily to deficiencies in nuclear effective interactions, which can be removed but not easily.

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