On the sensitivity of nuclear clocks to new physics

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The recent demonstration of laser excitation of the ≈ 8 eV isomeric state of thorium-229 is a significant step towards a nuclear clock. The low excitation energy likely results from a cancellation between the contributions of the electromagnetic and strong forces. Physics beyond the Standard Model could disrupt this cancellation, highlighting nuclear clocks' sensitivity to new physics. Accurate predictions of the different contributions to nuclear transition energies, and therefore of the quantitative sensitivity of a nuclear clock, are challenging. We improve upon previous sensitivity estimates and assess a "nightmare scenario," where all binding energy differences are small and the new physics sensitivity is poor. A classical geometric model of thorium-229 suggests that fine-tuning is needed for such a scenario. We also propose a d-wave halo model, inspired by effective field theory. We show that it reproduces observations and suggests the "nightmare scenario" is unlikely. We find that the nuclear clock's sensitivity to variations in the effective fine structure constant is enhanced by a factor of order 10^4 . We finally propose auxiliary nuclear measurements to reduce uncertainties and further test the validity of the halo model.

1. INTRODUCTION

Roughly 80% of the matter content of our Universe consists of dark matter (DM). Despite ample evidence for its existence from astrophysical and cosmological observations, little is known about its nature, and it is considered to be one of the greatest mysteries of contemporary physics. Theories of ultralight dark matter (ULDM) bosons (scalar or pseudo-scalar) provide us with arguably the simplest explanation for its nature. Well-motivated models of ULDM include the axion [1–5] of quantum chromodynamics (QCD), the dilaton [6] (though see Ref. [7]), the relaxion [8, 9], and possibly other forms of Higgs-portal models [10]. Finally, it was recently shown that the Nelson–Barr framework that also addresses the strong-CP problem, leads to a viable ULDM candidate [11]. All of these models predict that the ULDM would couple dominantly to the Standard Model (SM) QCD sector, the quarks and the gluons, leading to oscillations of nuclear parameters [12–14]. These models would also lead to subdominant coupling to the QED sector via time variation of $\alpha_{\rm em}$, the fine structure constant. Scalar ULDM generically couples linearly to the hadron masses

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(see [15] for a recent review), whereas pseudo-scalars (axions) couple quadratically [16] (though see Ref. [17, 18]). Furthermore, one can construct a broad class of natural ULDM models where the leading DM interaction with the SM fields is quadratic [19]. All of these lead to oscillation of the nuclear/hadronic parameters.

Variations of SM parameters can be searched for by comparing the rates of two clocks (e.g., quantum transitions or resonators) that exhibit different dependence on the parameters in question [6, 14, 20]. Laboratory limits on these variations have been obtained from various clock-comparison experiments based on atomic or molecular spectroscopy as well as cavities and mechanical oscillators. However, these experimental probes mostly rely on electronic transitions, whereas their sensitivity to changes in the nuclear sector is largely suppressed. Hyperfine transitions and mechanical oscillators, (Cs clock, hydrogen maser, quartz oscillator) [21–26], which are sensitive to variation of the nuclear parameters, do not reach the accuracy and stability of optical clocks. In optical clocks nuclear properties enter via hyperfine structure and the reduced mass, but their relative contributions are typically only of order 10^{-6} and 10^{-5} , respectively. The contributions from the oscillation of the charge radius, is around 10^{-3} [27]. Rovibrational transitions in molecules promise an $\mathcal{O}(1)$ sensitivity to a modulation of nuclear parameters [28, 29], although current constraints only exist at modulation frequencies above $10\,\mathrm{Hz}$ [30].

This is one of two main reasons for why a nuclear clock, which precisely monitors an ultra-narrow nuclear transition, could lead to a quantum leap in ULDM searches, [31–34]. The only isotope known to possess a suitable clock-nuclear transition is ²²⁹Th, which features an isomeric state, ^{229m}Th, a mere 8 eV above the ground state, low enough to be excitable with a laser [35, 36] (for illustration see Fig. 1). In fact, laser excitation of this transition has recently been reported for the first time [37–39]. This constitutes a major breakthrough on the way towards a nuclear clock, which is hoped to surpass the frequency stability of even the best atomic clock, given that the nucleus is better shielded from environmental noise than the electron shell. Regarding searches for physics beyond the SM, line-shape analysis of the ²²⁹Th data would lead to world-record sensitivity already now, well before a nuclear clock is going to be realized [40].

The second reason for why the nuclear clock might be extremely sensitive to the presence of new physics is due to an accidental cancellation between the nuclear energy shift and the electromagnetic energy shift compared to the ground state, which results in the observed small transition energy. New physics that couples differently to either of these contributions disrupts this cancellation. A nuclear clock is therefore believed to have spectacular sensitivity to certain classes of physics beyond the SM, naively being of the order of MeV/ $10\,\mathrm{eV}\sim10^5$. The sensitivity of a nuclear clock to physics beyond the SM has been explored in a number of papers (see for example [41–47]). Recent reviews can be found in Refs. [15, 48, 49].

However, to accurately quantify this sensitivity, the degree of fine-tuning in the transition energy (or, in other words, the absolute magnitude of the electromagnetic or nuclear energy difference between the ground state and the isomer) needs to be known. This is hindered by intrinsic imperfection in all models of atomic nuclei. At the moment, as we will see below, even a "nightmare scenario" where *no* cancellation occurs (and the electromagnetic and nuclear energy differences happen to be at the eV scale individually) cannot be ruled out. This would leave the nuclear clock with a disappointing enhancement factor of $\mathcal{O}(1)$.

Our goal in the present paper is to quantify how likely this nightmare scenario is. We do so by calculating the Coulomb energy difference between the ground state and the isomer of ²²⁹Th first in a classical, geometric, model of the nucleus, parameterized by its charge radius, quadrupole and higher moments, as well as the skin thickness (Section 2.1). We then derive similar results using a quantum halo model, in which ²²⁹Th is described as a ²²⁸Th core orbited by a halo neutron, and the two states differ in the spin alignment of the halo neutron (Section 2.2). Finally, in Section 3, we conclude and propose a number of auxiliary measurements and further steps that could shed more

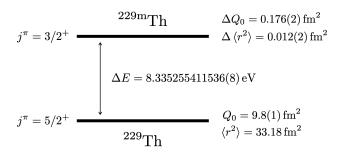


FIG. 1. Illustration of nuclear level properties, namely excitation energy ΔE [35, 36], intrinsic electric quadrupole momentum Q_0 [39, 50] and mean squared charge radius $\langle r^2 \rangle$ [42, 50, 51], of the almost-degenerate ground-state ²²⁹Th and isomer ^{229m}Th.

light on the likelihood of the nightmare scenario and the sensitivity of a nuclear clock to physics beyond the SM.

2. THE ²²⁹Th NUCLEUS

²²⁹Th is a heavy nucleus. This trivial fact makes its modeling from first principles problematic. The problem intensifies when considering the isomeric state, whose energy difference with the ground state, $\Delta E = 8.335\,255\,411\,536(8)\,\mathrm{eV}$ [39], lies far below typical nuclear physics scales. As mentioned before, the presumed explanation for this unnaturally low scale is a cancellation between the electromagnetic contribution, ΔE_{em} , and the nuclear contribution, ΔE_{nuc} , to the transition energy,

$$\Delta E = \Delta E_{\rm em} + \Delta E_{\rm nuc} \,, \tag{1}$$

where very naively we expect $|\Delta E_{\rm em}| \sim |\Delta E_{\rm nuc}| \gg \Delta E$. Physics beyond the SM may affect one of these contributions, but not the other, thereby breaking the fine-tuned cancellation.

The conventional lore is that this implies a sensitivity that is enhanced compared to the sensitivity of an optical lattice clock by a factor of $|\Delta E_{\rm em}|/\Delta E \simeq |\Delta E_{\rm nuc}|/\Delta E$. To compute the enhancement factor, determine the sensitivity of a ^{229m}Th nuclear clock to new physics, and interpret measurements in this context, it is necessary to determine $\Delta E_{\rm em}$ independently. As $\Delta E_{\rm em}$ is not an observable, and at present cannot be computed from first principles, this requires modelling.

More precisely, if physics beyond the SM manifests itself as an effective variation of the strong coupling constant, $\delta \alpha_s$, and/or an effective variation of the electromagnetic coupling constant, $\delta \alpha_{\rm em}$, (for instance due to dark matter oscillations), we can use Eq. (1) to write the corresponding variation of the transition energy as

$$\frac{\delta(\Delta E)}{\Delta E} = \frac{1}{\Delta E} \left(\frac{\partial \Delta E_{\rm em}}{\partial \alpha_{\rm em}} \delta \alpha_{\rm em} + \frac{\partial (\Delta E_{\rm em} + \Delta E_{\rm nuc})}{\partial \alpha_s} \delta \alpha_s \right), \tag{2}$$

where in Eq. (2) we have used the fact that $\partial(\Delta E_{\rm em} + \Delta E_{\rm nuc})/\partial\alpha_{\rm em} = \partial\Delta E_{\rm em}/\partial\alpha_{\rm em}$. In case of a time varying background they would become accessible for quantum sensors, contrary to $\Delta E_{\rm em}$ and $\Delta E_{\rm nuc}$ themselves.

Dark matter-induced variations of $\alpha_{\rm em,s}$ are typically of the form $\delta\alpha_{\rm em,s} = \alpha_{\rm em,s}(1 + \mathcal{F}(t)g_{\rm em,s})$, where $g_{\rm em,s}$ denotes the dark matter coupling strength to either the electromagnetic or strong sector of the SM, while $\mathcal{F}(t)$ is a function which depends on the dark matter energy density and mass, with the latter setting the frequency at which $\mathcal{F}(t)$ oscillates.

In the following we focus on the computation of the electromagnetic enhancement factor, defined as

$$K_{\rm em} \equiv \frac{1}{\Delta E} \frac{\partial \Delta E_{\rm em}}{\partial \log \alpha_{\rm em}} \simeq \frac{\Delta E_{\rm em}}{\Delta E} \,,$$
 (3)

where in the last equality we have assumed that $\Delta E_{\rm em}$ depends linearly on $\alpha_{\rm em}$. Any other power-law dependence will give an order-one correction which is irrelevant for the scope of this work. $K_{\rm em}$ arises naturally as the quantity of interest for dark matter candidates which couple to the electromagnetic sector; however, as explained in the introduction, such candidates are typically well constrained by other probes. But some of the most appealing and well-motivated dark matter candidates couple to the strong sector, and it is therefore of great interest to compute the corresponding enhancement factor $K_s = K_s^{\rm em} + K_s^{\rm nuc}$ related to variations of the effective value of α_s . The effect of such variations is, unfortunately, very difficult to model. Nevertheless, we notice that as long as $\Delta E_{\rm em}$ has a polynomial dependence on α_s (this dependence can come, for example, from the variation of the nuclear radius with α_s , see [27] for a relevant discussion), we expect

$$K_s^{\rm em} \equiv \frac{1}{\Delta E} \frac{\partial \Delta E_{\rm em}}{\partial \log \alpha_s} \sim \beta \frac{\Delta E_{\rm em}}{\Delta E} \sim \beta K_{\rm em} \,, \tag{4}$$

where we introduced an overall factor β , which we expect to be of order one, but which can slightly change for different functional dependencies of $\Delta E_{\rm em}$ on α_s . Barring fine-tuning cancellations between $K_s^{\rm em}$ and the analogous quantity for the nuclear energy, $K_s^{\rm nuc} \equiv \frac{1}{\Delta E} \frac{\partial \Delta E_{\rm nuc}}{\partial \log \alpha_s}$, we expect our computation of $K_{\rm em}$ to be a good proxy for K_s as well, and therefore our conclusions to apply also to dark matter models which couple to the strong sector. This statement can be invalidated only if the functional dependence of $\Delta E_{\rm em}$ and $\Delta E_{\rm nuc}$ on α_s is exactly the same.

We now turn to the actual determination of $\Delta E_{\rm em}$ and its variation with $\alpha_{\rm em}$ and define the corresponding enhancement factor as

$$K \equiv |K_{\rm em}| \,. \tag{5}$$

Recent studies on this topic have modelled the ²²⁹Th nucleus using a purely geometric model [42, 52]. This is a classical model, in which the nucleus is described as a three-dimensional body with some charge distribution – in the simplest case a homogeneously charged sphere or ellipsoid. Its electrostatic energy can then be derived easily using standard methods from elementary electrodynamics. The energy difference between the ground state and the isomer is interpreted as due to a change in the shape of the nucleus; and the shapes of the two states are modelled from observables, notably the measured nuclear charge radius and electric quadrupole moment.

However, the geometrical model has several severe shortcomings. First, its classical nature neglects a possible quantization of nuclear deformations. Second, it only assesses the direct (Hartree) contribution to the electrostatic energy, neglecting exchange (Fock), vacuum polarization, and spin-orbit coupling terms [53]. These are typically small compared to the direct contribution in absolute terms, but since we are interested in electromagnetic energy differences, they may nevertheless be important. In particular, the excitation from the ground state (spin 5/2) to the isomeric state (spin 3/2) can be interpreted as a single neutron spin flip. In this case, the change in the spin-orbit term, which is the smallest of the four corrections in absolute terms [53], might even dominate the electromagnetic contribution to the excitation energy. (Note that even though the spin-orbit term is small, it is still much larger than the observed energy difference of order $8 \, \text{eV}$.)

This motivates an alternative description of the ²²⁹Th nucleus: the so-called halo model, in which ²²⁹Th is described as a monolithic spin-0 ²²⁸Th nucleus orbited by a relatively loosely bound "halo neutron". Models with one or several such halo nucleons have been applied successfully to

a number of nuclei, especially away from the valley of stability and near the neutron and proton driplines [54, 55]. In the case of 229 Th, a halo model is supported by the relatively smaller neutron separation energy ($S_n = 5.2567(26)$ MeV) in the ground state of 229 Th compared to the ground state of 228 Th (7.1052(23) MeV). A similar difference cannot be found comparing the proton separation energies in the ground states of 229 Th and 228 Th: 6.5981(28) MeV and 6.3676(21) MeV, respectively [56, 57]. The very similar charge radii of 228 Th (5.7488(152) fm) and 229 Th (5.7557(143) fm) lend support to the halo model in which the core is 228 Th and the difference in the charge radii of 228 Th and 229 Th is mainly due a recoil effect that is suppressed by the inverse mass number [54]. Given that the ground state of 228 Th has zero spin, the spins of the 229 Th ground state and 229 mTh isomer can be understood if the halo neutron is in a d-wave state; the ground state and the isomer then correspond to the two spin orientations of that neutron. Note, however, that the description in terms of a halo model is not supported by the nuclear shell model, in which the neutron valence shell is the $2g_{9/2}$ orbital containing three valence neutrons which moreover have the "wrong" angular momentum.

In the following, we investigate the predictions of both the geometric model and the halo model quantitatively.

2.1. The classical geometric model

In spite of its aforementioned shortcomings, the geometric model of the 229 Th nucleus has been widely adopted in the literature, including in several studies exploring the potential of nuclear clocks to look for new physics [42, 52]. We therefore study this model first, advancing it beyond previous calculations. Our goal is to compute the electromagnetic energy difference, $\Delta E_{\rm em}$ between the ground state and the isomer of 229 Th. Doing so at the required level of $\sim 8\,{\rm eV}$ is considered absurd in nuclear physics, and we do not claim to achieve this either. Instead, our aim is to estimate a preferred range of $\Delta E_{\rm em}$, and thereby to answer the following two questions:

- 1. What is the expected magnitude of $\Delta E_{\rm em}$, and therefore of the enhancement factor $\Delta E_{\rm em}/\Delta E$ (with $\Delta E \sim 8\,{\rm eV}$) benefiting searches for new physics?
- 2. How likely is a "nightmare scenario", where $\Delta E_{\rm em}$ is accidentally close to zero, so that no fine-tuned cancellation is required to explain the smallness of ΔE , and new physics searches would not benefit from an enhancement, or even suffer a suppression?

Our starting point is the nuclear charge density, which we describe with a Woods–Saxon distribution [58]:

$$\rho(r,\theta) = \frac{\rho_0}{1 + \exp\left(\frac{r - R(\theta)}{z}\right)},\tag{6}$$

where z is the "surface thickness" of the nucleus, R is its "radius" and the reference density ρ_0 is determined by the normalisation condition

$$Ze = \int d^3 \mathbf{r} \, \rho(r, \theta), \tag{7}$$

with e the electric charge unit, and Z = 90 for thorium. We model non-sphericity of the nucleus through an angular dependence in R, namely

$$R(\theta) = R_0 \left[1 + \beta_2 Y_{20}(\theta) + \beta_3 Y_{30}(\theta) + \beta_4 Y_{40}(\theta) + \dots \right], \tag{8}$$

where R_0 is the scale radius, the $Y_{lm}(\theta, \phi)$ denote spherical harmonics, and β_2 , β_3 , and β_4 are the coefficients of the quadrupole, octupole, and hexadecapole, respectively. We neglect higher multipole moments in this work. Assuming azimuthal symmetry, we have set the magnetic quantum number m to zero, thereby making sure that R depends only on the polar angle θ , not on the azimuthal angle ϕ . Note that β_3 and β_4 are not constrained by experiments yet, contrary to β_2 , but they all impact $\Delta E_{\rm em}$.

Given the density profile, we can compute the two quantities which are accessible experimentally, namely the mean squared charge radius

$$\langle r^2 \rangle \equiv \frac{1}{eZ} \int d^3 \mathbf{r} \, r^2 \rho(r, \theta) \,,$$
 (9)

and the intrinsic quadrupole moment

$$Q_0 \equiv \int d^3 \mathbf{r} \, r^2 \rho(r, \theta) \left[3\cos^2(\theta) - 1 \right] \,. \tag{10}$$

(We use the notation Q_0 here to distinguish the intrinsic quadrupole moment from the spectroscopic quadrupole moment $Q_s = Q_0[(j(2j-1)]/[(j+1)(2j+3)]$, which is often the quantity that is reported in the experimental literature.) The measurements of $\langle r^2 \rangle$ and Q_0 fix two parameters of our model. In particular the scale radius R_0 depends mainly on $\langle r^2 \rangle = (5.7557(143) \, \text{fm})^2 \, [50, 51]$, while the parameter β_2 is closely related to the intrinsic quadrupole moment, $Q_0 = 9.8(1) \, \text{fm}^2 \, [50]$. For small $\beta_{2,3,4}$ one finds, $\langle r^2 \rangle \sim R_0^2$ plus small corrections due to the skin thickness $\mathcal{O}(z^2/R_0^2)$, whose typical value is $z \sim 0.5 \, \text{fm}$. Similarly, for small β_2 one can write Q_0 as an expansion in β_2 . In the following we do not assume these expansions and numerically solve for the various parameters of our model.

Note that Ref. [42] relates $\langle r^2 \rangle$ to β_2 (or equivalently Q_0) by taking a constant volume approach, that is, by assuming equal R_0 for the ground state and the isomer. Furthermore, [42] studies the impact of small β_3 values on the energy difference $\Delta E_{\rm em}$, but not the impact of β_4 . Our study does not assume a constant volume. We numerically scan over the parameters β_3 , β_4 , and Δz to carefully asses their combined impact on nuclear clock sensitivity.

We now turn towards the main result of this section, namely the calculation of the electromagnetic energy for both the ground state and the isomer of 229 Th. We approximate this with the direct Coulomb energy contribution

$$E_{\rm em} \simeq E_{\rm C}[\langle r^2 \rangle, Q_0, z, \beta_3, \beta_4] = \frac{1}{2} \int d^3 \mathbf{r} \, d^3 \mathbf{r}' \, \frac{\rho(r, \theta) \, \rho(r', \theta')}{|\mathbf{r} - \mathbf{r}'|}. \tag{11}$$

The integral over the azimuthal angles can be evaluated analytically as the charge density does not depend on these angles. The four remaining integrals, however, must be done numerically. We show the results in Figs. 2 and 4.

In Fig. 2 we plot the enhancement factor K as a function of the relative quadrupole moment difference between the excited state and the ground state of 229 Th, $\Delta Q_0/Q_0$, for various combinations of $\beta_{3,4}$. We find that the "nightmare scenario" in which $K \simeq 0$, implying no enhanced sensitivity to new physics, is fairly unlikely. It would only be realized for very specific values of $\beta_{3,4}^{\rm gs,iso}$ of the ground state ("gs") and the isomer ("iso") chosen in such a way that the funnel region is aligned with the measured value of $\Delta Q_0/Q_0$ from Ref. [39] (vertical dark gray line in Fig. 2). In contrast, typical values of $K \sim 10^4$ – 10^5 are far more likely. To illustrate this point, we plot in Fig. 3 the enhancement factor K as function of $\beta_3^{\rm gs}$ and $\beta_3^{\rm iso}$ for $\beta_4^{\rm gs} = \beta_4^{\rm iso} = 0$ (left panel), and as a function of $\beta_4^{\rm gs}$ and $\beta_4^{\rm iso}$ for $\beta_3^{\rm gs} = \beta_3^{\rm iso} = 0$ (right panel). In both panels, ΔQ_0 has been fixed to the value measured in Ref. [39].

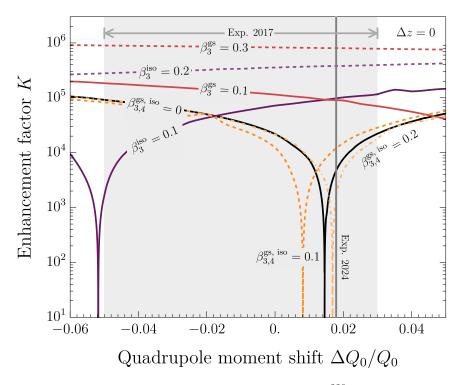


FIG. 2. The enhancement factor K benefiting new physics searches with 229 Th as a function of the quadrupole moment difference between the excited and ground states. The different colored lines correspond to different values of the higher electromagnetic multipole moments $\beta_{3,4}^{\rm gs,iso}$ of the ground state ("gs") and the isomer ("iso"), cf. Eq. (8). (The labels give only the multipole moments which are chosen different from zero.) The vertical gray line indicates the latest, very precise, measured value of $\Delta Q_0/Q_0$ [39], while the wide shaded gray band corresponds to the 1σ uncertainty from previous measurements [50]. We see that for specific values of $\Delta Q_0/Q_0$ and the values of $\beta_{3,4}^{\rm gs,iso}$, the K-factor may be drastically smaller than 10^5 .

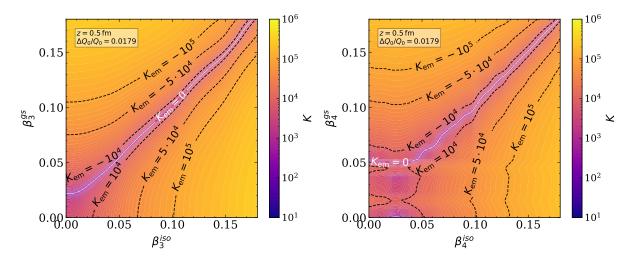


FIG. 3. The enhancement factor for new physics searches with 229 Th ("K-factor") as a function of the higher electrostatic multipole moments β_3 (left) and β_4 (right) of the ground state ("gs") and the isomer ("iso"). We see that K is typically of order 10^4 – 10^5 , except for a narrow funnel region. In both plots we have fixed z=0.5 fm and all the other parameters to their median experimental values.

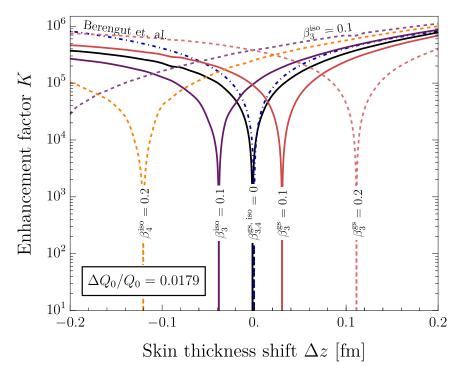


FIG. 4. The enhancement factor K as a function of the difference in the skin thickness between the excited and ground states of 229 Th. Colored lines correspond to various values of the higher electromagnetic multipole moments $\beta_{3,4}^{\rm gs,iso}$ of the ground state ("gs") and the isomer ("iso"), cf. Eq. (8). Similar to Figs. 2 and 3 we see that K can go to zero for specific values of Δz and $\beta_{3,4}^{\rm gs,iso}$, though for most values of these unknown parameters, K is of order 10^4 – 10^5 . The dot-dashed blue line shows the approximate expression for K from Eq. 7 of Ref. [52], which does not take into account the impact of $\beta_{3,4}$ and is a good approximation only for small Δz [59].

We finally discuss in Fig. 4 the impact of the neutron skin thickness, z, which we have so far chosen to be z=0.5 fm for both the ground state and the isomer. We see again that – depending on the values of Δz and $\beta_{3,4}^{\rm gs,iso}$ – K might be very small or zero. Note that the treatment of the skin thickness discussed in [52] is valid only for small Δz and does not simultaneously take into account the effects of $\beta_{3,4}$.

Finally, We explicitly checked that adding additional contributions to Eq. (11), for instance an exchange term describing Pauli blocking in the free Fermi gas approximation, has a minor effect and does not qualitatively change any of our conclusions. Including such terms would slightly change the values of $\beta_{3.4}^{\rm gs,iso}$ for which $K \ll 10^5$ by a small amount.

2.2. Th-229 as a Halo Nucleus

To describe 229 Th as a halo nucleus, we follow the halo Effective Field Theory (EFT) framework for shallow d-wave states developed in [60, 61], considering the ground state (j = 5/2) and the isomer (j = 3/2) which both have positive parity as a doublet resulting from the l = 2 coupling of the halo neutron to the 228 Th core system. We stress here that halo EFT should only be considered a model for the neutron– 228 Th system, not a proper EFT, as the separation between the low and high energy scales is marginal. If the expansion parameter is estimated as the ratio of the neutron separation energies of 229 Th $(S_n \approx 5.2 \,\text{MeV})$ and 228 Th $(S_n \approx 7.1 \,\text{MeV})$, it would be $\sqrt{5.2/7.1} \approx 0.86$. In addition, the predictivity of halo EFT is limited for d-wave nuclei as the

centrifugal barrier creates a strong dependence on short-distance (small r) effects and therefore on the overlap of the halo nucleon's wave function with the core. This is reflected in a leading-order dependence of most observables on counter-terms whose exact magnitude depends on the core—halo interaction model.

However, d-wave halo EFT suggests that the neutron-halo doublet states, j = 3/2 and j = 5/2, are degenerate at leading order, and that therefore the differences between their charge radii, quadrupole moments, etc., vanish at leading order [60, 61]. Thus, we develop here a model, inspired by halo EFT, that focuses on these differences, motivated by the nature of the isomeric transition. We begin by computing the two quantities to which we have experimental access, namely the mean squared charge radius and the quadrupole moment. Within our halo model, the charge density of the ground and excited states are identical, except for a difference stemming from the spin-orbit interaction between the halo neutron's spin and its l = 2 orbital angular momentum. This spin-orbit contribution to the charge density is given by [62]

$$\rho_{SO} = \frac{\mu_n}{2m_n^2} i \sigma_{\alpha\beta} \cdot \left[(\nabla \Phi_{\alpha}^{\dagger}) \times (\nabla \Phi_{\beta}) \right], \tag{12}$$

where $\mu_n = -1.91$ is the magnetic moment of the neutron in units of the nuclear magneton, Φ is the (non-relativistic 2-component) neutron spinor and $\alpha, \beta = 1, 2$ are spinor indices. With ρ_{SO} at hand we can compute the mean squared charge radius and the quadrupole moment, in analogy to our calculation from Section 2.1 for the geometric model.

We start with the contribution from the spin-orbit charge density to the mean squared radius $\Delta \langle r^2 \rangle$. Following Ref. [62], it is given by

$$\langle r^2 \rangle_{SO} = \frac{1}{Z} \int r^2 \rho_{SO} d^3 \mathbf{r} = -\frac{\mu_n}{m_n^2 Z} (\kappa + 1), \qquad (13)$$

where

$$\kappa = \begin{cases} l & \text{for } j = l - \frac{1}{2} \\ -(l+1) & \text{for } j = l + \frac{1}{2} \end{cases}$$
(14)

Then, for the difference between the isomer and the ground state we obtain

$$\Delta \langle r^2 \rangle_{SO} \equiv \langle r^2 \rangle_{SO}^{iso} - \langle r^2 \rangle_{SO}^{gs} = 0.0047 \,\text{fm}^2$$
 (15)

This value is smaller than the measured $\Delta \langle r^2 \rangle = 0.012(2) \, \text{fm}^2$ [50] by only a factor of ~ 2 , which we consider excellent agreement given the inherent uncertainties to the halo model.

For the intrinsic nuclear quadrupole moment,

$$Q_{SO} = \int r^2 (3\cos^2\theta - 1)\rho_{SO} d^3\mathbf{r}, \qquad (16)$$

we find $Q_{\rm SO}^{\rm gs}=8\mu_n/(5m_n^2)$ for the ground state, and $Q_{\rm SO}^{\rm gs}=-3\mu_n/(5m_n^2)$ for the isomer. Using again $\mu_n=-1.91$, we find

$$Q_{\rm SO}^{\rm iso} - Q_{\rm SO}^{\rm gs} = 0.185 \,\text{fm}^2\,,$$
 (17)

in astonishingly good agreement with the latest experimental value [39]

$$(Q^{\rm iso} - Q^{\rm gs})_{\rm exp} = 0.175525(6) \,\text{fm}^2.$$
 (18)

We consider this a further validation of the halo model for 229 Th. We also notice that the computations of $\Delta \langle r^2 \rangle_{\rm SO}$ and $Q_{\rm SO}^{\rm iso} - Q_{\rm SO}^{\rm gs}$ are *not* sensitive to UV physics, i.e., insensitive to the

structure of the wave-function near the origin. The main assumption in these calculations is that the contribution originates in single nucleons [62], i.e., consistent with a halo model [54]. This leaves room for possible renormalization of the halo-neutron magnetic moment, which offers an explanation for the $\approx 50\%$ deviation from experiment.

Having shown that the halo model gives sensible results for the mean squared charge radius and the quadrupole moment, we now compute the spin-orbit contribution to the binding energy of the halo neutron [63]

$$E_{SO} = \frac{e\,\mu_n}{2m_n^2} \frac{1}{2} \left[j(j+1) - l(l+1) - \frac{3}{4} \right] \int_0^\infty \left[\frac{[u(r)]^2}{r} \frac{dV_C}{dr} \right] dr \,, \tag{19}$$

where l=2 and j=5/2 (ground state) or 3/2 (isomer) are its angular momentum quantum numbers, $V_{\rm C}(r)$ is the Coulomb potential of the ²²⁸Th core, and u(r) is the excess neutron's radial d-wave function [64]:

$$u(r) = A(r)e^{-\gamma r} \left(1 + \frac{3}{\gamma r} + \frac{3}{(\gamma r)^2}\right).$$
 (20)

In this expression, $\gamma \equiv \sqrt{2m_n E_B}$, $E_B = 5.2 \,\mathrm{MeV}$ is the binding energy, and A(r) is determined by short-range physics. A(r) has a weak dependence on r, and it asymptotically converges to a constant A at large r, that is therefore called the asymptotic normalization constant (ANC). At leading order in halo EFT, A is taken to be fully independent of r, and depends on the UV cutoff scale, which is what we assume in the following. As usual in EFTs, the behavior of the ANC at short distances should be fixed from additional experimental constraints, see the discussion in Section 3. Since the neutron separation energy for the ground state of 229 Th is expected to be almost the same as for the isomer, a good assumption is that u(r) is also the same for j = 5/2 and j = 3/2. After all, these quantum numbers are just a result of the spin-orbit coupling for fixed l = 2, and we treat the spin-orbit potential as a small perturbation.

In order to estimate $E_{\rm SO}$ from Eq. (19), we also need to specify the Coulomb potential, $V_{\rm C}(r)$, which we derive from the nuclear charge density distribution. As the halo-neutron radial wave function is dominated by the length scale γ^{-1} , i.e., few Fermi, much larger than the UV length-scale, the charge density can be approximated by a Woods–Saxon form [65], see Eq. (6). Since for heavy nuclei $R_0 \gg z$, we can further approximate the charge density $\rho(r) \approx \frac{3}{4\pi R_0^3} Ze \Theta(R_0 - r)$, leading to

$$V_{\rm C}(r) = \begin{cases} \frac{Ze}{2R_0} \left(3 - \left(\frac{r}{R_0}\right)^2\right) & r < R_0 \\ \frac{Ze}{r} & r > R_0 \end{cases}$$
 (21)

Thus, the universal property $\rho \approx \text{constant}$ leads to $dV_{\rm C}/dr \propto r$, which conveniently cancels the UV sensitivity of the integral in Eq. (19), i.e.,

$$\int_0^\infty \frac{[u(r)]^2}{r} \frac{dV_{\rm C}}{dr} dr = \frac{Ze}{R_0} \left(\frac{1}{R_0^2} \int_0^{R_0} [u(r)]^2 dr + \int_{R_0}^\infty R_0 [u(r)]^2 \frac{dr}{r^3} \right). \tag{22}$$

Thus, $\int_0^\infty \frac{(u(r))^2}{r} \frac{dV_C}{dr} dr$ is not divergent. Both integrals on the right-hand side are finite, the first one due to the normalization of u(r), and the second because it is controlled by the free d-wave solution, cf. Eq. (20). For the parameters of ²²⁹Th, the first integral dominates. In order to evaluate this integral we introduce a short-distance cutoff, l, to regularize the divergence of the integrand at $r \to 0$, and we assume a constant A(r), constrained by the normalization condition on u(r). We find that the integral is almost independent of l for values $l \le 4$ fm. Numerically, we then obtain

$$\Delta E_{\rm SO} = E_{\rm SO}|_{j=5/2} - E_{\rm SO}|_{j=3/2} \approx 144 \, p \, \text{keV} \,,$$
 (23)

where the order-one factor p is a function of A and l. A more complete nuclear model would predict a specific form for A(r), eliminating the need for a regulator, and thereby determining p. Intuitively, p is related to the probability of finding the halo neutron inside the nucleus.

Summarizing, we find the contribution of the spin-orbit interaction to $\Delta E_{\rm em}$ to be of order 100 keV, which corresponds to an enhancement factor $K \approx 10^4$ for new physics searches using nuclear clocks.

3. SUMMARY AND OUTLOOK

In this work we have studied how the sensitivity of a 229 Th nuclear clock to new physics depends on nuclear modelling. On the one hand, we have shown that within a classical geometric model of the 229 Th nucleus, which is widely used in the literature, a "nightmare scenario" in which the sensitivity goes to zero is possible, although it requires fine-tuning of the model parameters at the per cent or per mille level. On the other hand, we have presented a more realistic quantum halo model, in which an approximately unpaired neutron of 229 Th is loosely bound to a 228 Th spin-0 core. The neutron is in a d-wave state, with orbital angular momentum l=2. We have validated this model against the experimentally measured differences of charge radii and quadrupole moments of the 229 Th ground state and of the isomer 229 mTh. The model correctly predicts these differences to be close to zero. Within the halo model, the "nightmare scenario" is never realized and the enhancement factor $K_{\rm em}$ for new physics searches is always $\gtrsim 10^4$.

Our work suggests multiple directions of future research. It is clear that the main obstacle to an accurate determination of the enhancement factor is the nuclear model, which has multiple unknown parameters. In the future, we hope it will be possible to further refine and verify the halo model using in particular neutron capture experiments. The amplitude of neutron capture in d-wave halos is proportional to the asymptotic normalization constant A. Thus, a neutron capture experiment can give a quantitative constraint on the probability of finding the halo-neutron inside the core, which governs the size of the spin-orbit contribution to the electromagnetic interaction. In addition, we have assumed that A is identical for the ground state and for the isomer. This assumption can, in principle, be verified by measuring the neutron capture cross section, $\sigma_{\rm cap}$, for both states. Halo EFT predicts $\sigma_{\rm cap}^{\rm iso} = \frac{2}{3}\sigma_{\rm cap}^{\rm gs}$ [60].

Moreover, it is important to confirm the latest results for $\Delta Q_0/Q_0$ [39], and to possibly also improve the determination of $\Delta \langle r^2 \rangle$. In addition, it is highly desirable to devise further tests of the shape of the nucleus, sensitive to the higher-order multipoles $\beta_{3,4}$ and the skin thickness z. These quantities are crucial for determining the enhancement factor within the classical geometric model, which – despite the shortcomings we have stressed several times – is still of interest and represents an alternative to the d-wave halo model.

Finally, we have argued in the introduction to Section 2 that $K_{\rm em} \sim K_s$, and that therefore our results apply both to new physics coupled to the electromagnetic sector and to new physics coupled to the strong sector. We believe this to be true unless the electromagnetic and nuclear energy differences between the ground and excited states of thorium-229 conspire to have the exact same functional dependence on α_s . Indeed, in EFT approaches to the expansion of nuclear forces in the QCD scale, the electromagnetic and strong contributions are predicted to have different dependence on this scale [55, 66]. However, it is key to verify this within concrete frameworks. We leave this and other exciting developments for future work.

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Appendix A: Spin-Orbit Contribution to the quadrupole moment

Here we provide details on the computation of the spin-orbit contribution to the intrinsic nuclear quadrupole moment for halo nuclei. In general, this contribution is

$$Q_{SO} = \int r^2 (3\cos^2\theta - 1)\rho_{SO} d^3\mathbf{r}.$$
 (A1)

Following the appendix of ref. [62], we split Q_{SO} into two pieces. The first one is

$$Q_{\text{SO}}^{(1)} = -\frac{3\mu_n}{2m_n^2} (\kappa + 1) \int d\cos\theta \, d\phi \, \Omega_{jlm}^{\dagger} \Omega_{jlm} \left(3\cos^2\theta - 1 \right), \tag{A2}$$

where

$$\Omega_{jlm} = \begin{pmatrix} C_{lm-\frac{1}{2},\frac{1}{2}\frac{1}{2}}^{jm} Y_l^{m-\frac{1}{2}} \\ C_{lm+\frac{1}{2},\frac{1}{2}-\frac{1}{2}}^{jm} Y_l^{m+\frac{1}{2}} \end{pmatrix}$$
(A3)

is the angular part of the spinor, and the C are Clebsch–Gordan coefficients relating the orbital angular momentum l and the spin to the total angular momentum j. In our case, l=2, j=5/2 (ground state) or 3/2 (isomer), and the choice of m is arbitrary as the corresponding phase factors drop out in $\Omega_{ilm}^{\dagger}\Omega_{jlm}$.

The second contribution to Q_{SO} is more involved and reads [62]

$$Q_{\text{SO}}^{(2)} = \frac{\mu_n}{2m_n^2} \int d\theta \, d\phi \, i \left[\cos \theta \left(\frac{\partial \Omega_1^{\dagger}}{\partial \theta} \frac{\partial \Omega_1}{\partial \phi} - \frac{\partial \Omega_1^{\dagger}}{\partial \phi} \frac{\partial \Omega_1}{\partial \theta} \right) \right. \\ \left. + \sin \theta e^{-i\phi} \left(\frac{\partial \Omega_1^{\dagger}}{\partial \theta} \frac{\partial \Omega_2}{\partial \phi} - \frac{\partial \Omega_1^{\dagger}}{\partial \phi} \frac{\partial \Omega_2}{\partial \theta} \right) \right. \\ \left. + \sin \theta e^{i\phi} \left(\frac{\partial \Omega_2^{\dagger}}{\partial \theta} \frac{\partial \Omega_1}{\partial \phi} - \frac{\partial \Omega_2^{\dagger}}{\partial \phi} \frac{\partial \Omega_1}{\partial \theta} \right) \right. \\ \left. - \cos \theta \left(\frac{\partial \Omega_2^{\dagger}}{\partial \theta} \frac{\partial \Omega_2}{\partial \phi} - \frac{\partial \Omega_2^{\dagger}}{\partial \phi} \frac{\partial \Omega_2}{\partial \theta} \right) \right] (3\cos^2 \theta - 1).$$
 (A4)

Here, we have omitted the indices jlm on Ω_{jlm} to shorten the notation. The subscripts 1, 2 refer to the two components of the spinor. The integrals in Eqs. (A2) and (A4) can be performed analytically, and the total spin-orbit contribution to the quadrupole moment,

$$Q_{SO} = Q_{SO}^{(1)} + Q_{SO}^{(2)} \tag{A5}$$

is found to be $Q_{SO}^{gs} = 8\mu_n/(5m_n^2)$ for the ground state, and $Q_{SO}^{gs} = -3\mu_n/(5m_n^2)$ for the isomer, as written in the main text.

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