Nuclear structure corrections to the Lamb shift in $\mu^3$He$^+$ and $\mu^3$H

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Measuring the 2S-2P Lamb shift in a hydrogen-like muonic atom allows one to extract its nuclear charge radius with a high precision that is limited by the uncertainty in the nuclear structure corrections. The charge radius of the proton thus extracted was found to be 7σ away from the CODATA value, in what has become the yet unsolved “proton radius puzzle”. Further experiments currently aim at the isotopes of hydrogen and helium: the precise extraction of their radii may provide a hint at the solution of the puzzle. We present the first ab initio calculation of nuclear structure corrections, including the nuclear polarization correction, to the 2S-2P transition in $\mu^3$He$^+$ and $\mu^3$H, and assess solid theoretical error bars. Our predictions reduce the uncertainty in the nuclear structure corrections to the level of a few percents and will be instrumental to the on-going $\mu^3$He$^+$ experiment. We also support the mirror $\mu^3$H system as a candidate for further probing of the nucleon polarizabilities and shedding more light on the puzzle.

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I. INTRODUCTION

The root-mean-square (RMS) charge radius of the proton $r_p \equiv \sqrt{\langle r_p^2 \rangle}$ was recently determined with unprecedented precision from laser spectroscopy measurements of 2S-2P transitions in muonic hydrogen $\mu$H, where the electron is replaced by a muon [1, 2]. The extracted $r_p$ differs by 7σ from the CODATA value [3], which is based in turn on many measurements involving electron-proton interactions. This discrepancy between the ‘muonic’ and ‘electronic’ proton radii ($r_p(\mu^-)$ and $r_p(e^-)$, respectively) is known as the “proton radius puzzle,” and has attracted much attention (see, e.g., Ref. [4] for an extensive review and Ref. [5] for a brief summary of current results and ongoing experimental effort). In an attempt to solve the puzzle, extractions of $r_p(e^-)$ from the ample electron-proton (ep) scattering data have been reanalyzed by, e.g., Refs. [6–9], while several planned experiments aim to re-measure ep scattering in new kinematic regions relevant for the puzzle [10, 11]. $r_p$ extracted from electronic hydrogen is also being reexamined, both theoretically [12] and experimentally [13–15], as well as the Rydberg constant [15, 16], which is relevant for several radius extraction methods. A few of the theoretical attempts to account for the discrepancy between $r_p(e^-)$ and $r_p(\mu^-)$ include new interactions that violate lepton universality [17–19] and novel proton structures [20–24]. Yet the puzzle has not been solved. Answers may be provided (see, e.g. Refs. [25, 26]) by a planned experiment at PSI [27] to scatter electrons, muons, and their antiparticles off the proton using the same experimental setup.

Alternatively, it will be insightful to study whether the puzzle also exists in other light nuclei, and whether it depends on the atomic mass $A$, charge number $Z$, or the number of neutrons $N$. In particular, the CREMA collaboration plans to extract high-precision charge radii from Lamb shift measurements that were recently performed in several hydrogen-like muonic systems [5, 28], namely, $\mu$D, $\mu^3$He$^+$, and $\mu^4$He$^+$. These measurements may unveil a dependence of the discrepancy on the isospin of the measured nucleus and, in particular, probe whether the neutron exhibits a similar effect as the puzzling proton. To obtain some control over these issues, it is advisable that nuclei with different $N/Z$ ratios will be mapped out. It is the purpose of this Letter to perform an ab initio calculation of nuclear structure corrections (including nuclear polarization), with solid error estimates, for the $\mu^3$He$^+$ system and for its nuclear mirror, $\mu^3$H.

The Lamb shift [29] is the 2S-2P energy difference consisting of

$$\Delta E \equiv \delta_{\mathrm{QED}} + \delta_{\mathrm{FS}}(R_c) + \delta_{\mathrm{TPE}},$$

where, in decreasing order of magnitude, the three terms include: quantum electro-dynamics (QED) contributions from vacuum polarization, lepton self-energy, and relativistic recoil in $\delta_{\mathrm{QED}}$; finite-nucleus-size contributions in $\delta_{\mathrm{FS}}(R_c)$, where $R_c = \sqrt{\langle R^2 \rangle}$ is the nuclear RMS charge radius; and contributions from two-photon exchange (TPE) between the lepton and the nucleus in $\delta_{\mathrm{TPE}}$. The last term can be divided into the elastic Zemach term and the inelastic polarization term, i.e., $\delta_{\mathrm{TPE}} = \delta_{\mathrm{Zem}} + \delta_{\mathrm{pol}}$. Additionally, each of these terms is separated into contributions from nuclear ($\delta^A$) and nucleonic ($\delta^N$) degrees
of freedom, \( \delta_{\text{TPE}} = \delta_{\text{Zem}}^A + \delta_{\text{Zem}}^N + \delta_{\text{pol}}^A + \delta_{\text{pol}}^N \).

In light muonic atoms, \( \delta_{\text{CED}} \approx 10^2-10^3 \text{ meV} \) and is estimated from theory with a precision better than \( 10^{-3} \text{ meV} \) [30–33]. At leading order \( \delta_{\text{FS}}(R_e) = m_r^3(Z\alpha)^3 R_e^2 \), with \( m_r \) the reduced mass of the muon-nucleus system, while higher-order contributions are at the sub-percentage level [30]. The limiting factor for the attainable precision of \( R_e \) extracted from Eq. (1) is by far the uncertainty in \( \delta_{\text{TPE}} \). This was confirmed in two recent papers that reviewed the theory in \( \mu D \) [32], and in \( \mu^3 \text{He} \) and \( \mu^4 \text{He} \) [33]. Ref. [32] covers all the theoretical contributions to the Lamb shift in \( \mu D \), including a summary of recent efforts by several groups [34–37] to accurately obtain \( \delta_{\text{TPE}} \) in \( \mu D \) and reliably estimate its uncertainty, which comes out an order of magnitude larger than the uncertainties in the other terms. Ref. [33] details all the contributions for the two helium isotopes. Many terms are recalculated, not including the polarization correction \( \delta_{\text{pol}} \). For \( \mu^3 \text{He}^+ \), \textit{ab initio} nuclear calculations were recently applied in Ref. [38], improving on decades-old estimates of \( \delta_{\text{pol}} \). For three-body nuclei, the only calculations of \( \delta_{\text{pol}} \) are outdated; based on old and simplistic nuclear models, their results are either inaccurate [39] or imprecise [40], reinforcing the need for modern, accurate, \textit{ab initio} calculations for the three-body nuclei.

II. NUCLEAR STRUCTURE CONTRIBUTIONS

The nuclear Zemach term \( \delta_{\text{Zem}}^A \) enters Eq. (1) as the elastic nuclear-structure contribution to \( \delta_{\text{TPE}}^A \). This term is of order \((Z\alpha)^5\) and is defined as

\[
\delta_{\text{Zem}}^A = -\frac{m_r^4(Z\alpha)^5}{24} \langle r^3 \rangle_{(2)} ,
\]

where \( \langle r^3 \rangle_{(2)} \) is the 3rd nuclear Zemach moment\(^2\), Friar & Payne showed [43] that the first-order corrections in \( \delta_{\text{pol}}^A \) contain a part that cancels \( \delta_{\text{Zem}}^A \) exactly. Calculation of this part can thus be avoided, as was done in Ref. [34], providing only the sum \( \delta_{\text{TPE}}^A = \delta_{\text{pol}}^A + \delta_{\text{Zem}}^A \). However, following Refs. [35, 38, 44], we calculate explicitly all the parts of \( \delta_{\text{pol}}^A \), including the Zemach term, as detailed below. This is done in order to: (a) allow comparison with other values in the literature, and (b) provide theoretical support for the alternative way of extracting \( R_e \) from Eq. (1) where the Zemach term is phenomenologically parameterized as [30]

\[
\delta_{\text{Zem}}^A = C \times R_e^3 .
\]

As in Refs. [35, 38], the energy correction due to nuclear polarization is obtained as a sum of contributions

\[
\delta_{\text{pol}}^A = \left[ \delta_{D1}^A + \delta_{T}^A + \delta_{C}^A + \delta_{M}^A \right] + \left[ \delta_{D3}^{(1)} + \delta_{D3}^{(2)} \right] + \left[ \delta_{N}^{(1)} + \delta_{N}^{(2)} \right] .
\]

Detailed formulas pertaining to most of the terms in Eq. (4) are found in [38] and are not repeated here. The largest correction comes from the leading term, \( \delta_{D1} \), related to the electric dipole. To this we add relativistic longitudinal and transverse corrections \( \delta_{T}^A \) and \( \delta_{C}^A \), respectively, as well as Coulomb distortion corrections \( \delta_{M}^A \). Here we follow Ref. [35] and include in \( \delta_{D3} \) only the logarithmically enhanced term from the next order in \( Z\alpha \). We generalize the treatment in Ref. [35] of the magnetic term \( \delta_{M}^A \) by using the impulse approximation operator that includes the orbital angular momentum [45]. First-order corrections \( \delta_{D3}^{(1)} \) and \( \delta_{D3}^{(2)} \) are related to a proton-proton correlation term and to the 3rd nuclear Zemach moment, respectively. Finally, at the next order we have the monopole \( \delta_{Q}^{(0)} \), quadrupole \( \delta_{Q}^{(2)} \), and interference \( \delta_{D1D3}^{(2)} \) terms. All the above terms are calculated using point nucleons. Finite-nucleon-size (NS) corrections appear in Eq. (4) as \( \delta_{NS}^{(1)} = \delta_{R1}^{(1)} + \delta_{Z1}^{(1)} \) and \( \delta_{NS}^{(2)} \), which we elaborate on below.

III. NUCLEON-SIZE-CORRECTIONS

The TPE in the point-nucleon limit is expressed as the interaction of photons with the structureless charged protons, while the neutrons are ignored. In this limit, the point-proton density operator is

\[
\hat{\rho}_p(R) \equiv \frac{1}{2} \sum_{a=1}^{A} \delta(R - R_a) \frac{1 + r_a^3}{2} ,
\]

where \( r_a^3 \) is the isospin projection operator. When the finite nucleon sizes are considered, \( \hat{\rho}_p(R) \) must be convoluted with the proton’s internal charge distribution, and a similar convolution is applied to the point-neutron density operator

\[
\hat{\rho}_n(R) \equiv \frac{1}{N} \sum_{a=1}^{A} \delta(R - R_a) \frac{1 - r_a^3}{2} .
\]

Following Refs. [38, 44], we apply a low-momentum expansion for the nucleon form factors, parameterized here by their mean square charge radii, \( r_{n/p}^2 \equiv \langle r_{n/p}^2 \rangle \). We adopt \( r_n^2 = -0.1161(22) \text{ fm}^2 \) [46]. For the proton, we may use either \( r_p(\epsilon^-) = 0.8775(51) \text{ fm} \) [3] or \( r_p(\mu^-) = 0.84087(39) \text{ fm} \) [2]. In fact, until the “proton radius puzzle” is resolved (or when \( R_e \) and other properties of the nuclei under consideration are measured using

\[\footnote{\delta_{\text{Zem}}^A \text{ was derived by Friar [41] as the first-order } Z\alpha \text{ correction to } \delta_{\text{FS}}(R_e) \text{ and is called the ‘Friar’ term in Ref. [52].}}\]

\[\footnote{We refer only to charge-charge Zemach moments; for more details see, e.g., Ref. [42].}\]
The leading NS correction \( \delta^{(1)}_{NS} \) is the sum of nucleon-nucleon correlations in \( \delta^{(1)}_{R_1} \) and Zemach-like terms in \( \delta^{(1)}_Z \). The former is expressed as

\[
\delta^{(1)}_{R_1} = -\frac{n_f(Z\alpha)^5}{6} \int \int dR dR' |R - R'|(r_p^2(0)|\hat{\rho}_p(R)\hat{\rho}_p(R')|0) + \frac{N}{Z} r_n^2(0)|\hat{\rho}_n(R)\hat{\rho}_n(R')|0),
\]

which includes proton-proton (pp) and neutron-proton (np) correlations. It is an NS correction to the point-nucleon term \( \delta^{(1)}_{R_3} \) of Eq. (4) (the latter is denoted \( \delta^{(1)}_{R_{pp}} \) in Ref. [38]). For the calculation of Zemach-like terms using point-nucleons we define

\[
\langle r_i^1 \rangle_{(2)} = \int \int dR dR' |R - R'|^k (0|\hat{\rho}^1_i(R)|0)(0|\hat{\rho}_j(R')|0),
\]

with \( i, j \) denoting either \( p \) or \( n \). The 3rd nuclear Zemach moment is thus calculated as

\[
\langle r^3 \rangle_{(2)} = \langle r^3_{pp} \rangle_{(2)} + 4 \left[ r_p^2(r_{pp}^1)_{(2)} + \frac{N}{Z} r_n^2(r_{np}^1)_{(2)} \right],
\]

where the first term is the point-nucleon limit and the second is the (approximated) NS correction. Accordingly, the point-nucleon Zemach term \( \delta^{(1)}_{Z3} \) and its NS correction \( \delta^{(2)}_{ZNS} \) are obtained by inserting Eq. (9) into Eq. (2) and flipping the sign, i.e., \( \delta^{(1)}_{ZNS} \approx -\delta^{(1)}_{Z3} + \delta^{(1)}_{Z1} \).

The sub-leading NS correction \( \delta^{(2)}_{NS} \) is evaluated through a sum rule of the dipole response \(^3\)

\[
\delta^{(2)}_{NS} = -8\pi \frac{27}{27} n_f(Z\alpha)^5 \left[ r_p^2 - \frac{N}{Z} r_n^2 \right] \int_{\omega_{th}}^{\infty} d\omega \sqrt{\omega \frac{2m_r}{2m_r} S_D(\omega)}.
\]

Lastly, the nucleonic TPE correction \( \delta^{(3)}_{TPE} \) also enters Eq. (1). We defer the treatment of this hadronic contribution to a dedicated section below.

### IV. METHODS

Most of the above contributions can be written as sum rules of several nuclear responses with various energy-dependent weight functions [35, 38]. They were evaluated using the newly developed Lanczos sum rule method [47]. Ground-state observables of \(^3\)He and \(^3\)H, as well as Lanczos coefficients, were obtained using the effective interaction hyperspherical harmonics (EIHH) method [48, 49].

As only ingredients we employed in the nuclear Hamiltonian either one of the following state-of-the-art nuclear potentials: (i) the phenomenological AV18/UIX potential with two-nucleon [50] plus three-nucleon [51] forces; and (ii) the chiral effective field theory \( \chi \)EFT potential with two-nucleon [52] plus three-nucleon [53] forces.

It is of utmost importance to have realistic uncertainty estimates for our nuclear TPE predictions. These terms are the least well known in Eq. (1), and their uncertainties determine the attainable precision of \( R_c \) extracted from Lamb shift measurements. We considered many sources of uncertainty, namely: numerical; nuclear model; isospin symmetry breaking; higher-order nucleon-size corrections; missing relativistic and Coulomb-distortion corrections; higher multipoles, terms of higher-order in \( Z\alpha \); and the effect of meson-exchange currents on the magnetic contribution. Their individual and cumulative effect on \( \delta^{(4)}_{R_{pol}}, \delta^{(4)}_{Zem}, \) and \( \delta^{(4)}_{TPE} \) have been estimated and applied to the results given below. More details about these uncertainty estimates are given in the Supplementary Materials [54].

#### A. Results

We first compare a few observables we have calculated for the \(^3\)He and \(^3\)H nuclei with corresponding theoretical and experimental values available in the literature. In Table I we present the ground-state binding energy BE, charge radius \( R_c \), and magnetic moment \( \mu_g \), as well as the electric dipole polarizability \( \alpha_E \). In general, good agreement is found with other calculations.

Our results do not include isospin-symmetry breaking (ISB), except for the Coulomb interaction between protons in \(^3\)He. Calculations by other groups shown in Table I usually do not include ISB effects; notable exceptions are Ref. [56], which includes the \( T = 3/2 \) isospin channel in the ground-state wave function, and Ref. [55] which provides results either including or excluding it. One observes that including ISB alters BE by a few keV. In addition, the \(^3\)He BE, not used in the calibration of the Hamiltonians, is overestimated at a sub-percentage level, and this is slightly worsened when ISB is included. As discussed in Ref. [62], changes in BE shift the threshold of sum rules, affecting mostly sum rules with inverse energy dependence, such as \( \alpha_E \) discussed below. For the other observables in Table I, the estimated uncertainty stemming from ISB is \( \lesssim 1\% \).

Charge radii \( R_c \) shown in Table I are obtained from the calculated point-proton-distribution RMS radius \( R_p \) as [60, 66]

\[
R_p^2 = R^2 + r_v^2 + \frac{N}{Z} r_n^2 + \frac{3}{4m_r^2},
\]

where we omit contributions from the spin-orbit radius (negligible for s-shell nuclei) and meson-exchange currents. The last term in Eq. (11) is the Darwin-Foldy term, where \( m_r \) is the proton mass, taken from

\(^3\) The sign before \( r^2_p \) in Eq. (10) is corrected from Refs. [35, 38] and agrees with Ref. [57].
In Table I, we show only the experimental values. Our ground-state wave functions do not include the T = 3/2 channel. Our numerical uncertainties are not shown since they are smaller than one in the last decimal place. References labels correspond to: a Ref. [55], b Ref. [56], c Ref. [57], d Ref. [58], e Ref. [59], f Ref. [60], g Ref. [61], h Ref. [62], i Ref. [63], j Ref. [64], k Ref. [65] without/inclusion of the T = 3/2 channel, respectively; a Ref. [55] (which includes the T = 3/2 channel); a Ref. [56], b Ref. [57], c Ref. [58], d Ref. [59], e Ref. [60], f Ref. [61], g Ref. [62], h Ref. [63], i Ref. [64], k Ref. [65].

The electric dipole polarizability $\alpha_E$ is an inverse-energy-weighted sum rule of the dipole response and is therefore closely related to $\delta_{\text{Zem}}^A$. Our results are in agreement with previous calculations, especially the recent Ref. [62]. As in [38], $\alpha_E$ is found to be nuclear-model dependent. We provide first results for the unmeasured $\alpha_E$ of $^3$H with the AV18/UIX potential, which lies within the uncertainty estimates of [62].

We now turn to the Zemach terms, first listing available values in the literature. In Refs. [30, 31] Borič calculated $\delta_{\text{Zem}}$ following Friar [41], using a Gaussian distribution that fits the nuclear-charge radius obtained from electron experiments. The result $^{4,5}_{\text{AV18/UIX}} = -10.258(305)\text{ meV}$. Recently, Krutov et al. [33] repeated this calculation and obtained $\delta_{\text{Zem}}^A(\text{He}) = -10.28(10)\text{ meV}$. Alternatively, inserting the 3rd nuclear Zemach moment moment recently extracted from $e^{-\text{He}}$ scattering data [69] into Eq. (2) gives $\delta_{\text{Zem}}^A(\text{He}) = -10.87(27)\text{ meV}$. As explained above, all of these results should be compared with our calculation that uses $r_p(e^-)$ as input and yields $\delta_{\text{Zem}}^A(\text{He}) = -10.71(19)(16)\text{ meV}$, where the first uncertainty results from nuclear-model dependence and the second includes all other sources. Our result is in agreement with these references (based on comments made in Refs. [33, 69], we assume that the error-bars in Ref. [33] are not exhaustive). However, for the muonic systems considered here we use $r_p(\mu^-)$, which gives

$$\delta_{\text{Zem}}^A(\text{He})[r_p(\mu^-)] = -10.49(19)(16)\text{ meV}.$$  \hspace{1cm} (12)

We note that with the given error-bars this result is also in agreement with Refs. [31, 33, 69].

The use of Eq. (3) is adopted from Refs. [30, 31], where \( \mathcal{C}(\text{He}) = -1.35(4)\text{ meV fm}^{-3} \). The results of Ref. [69] can also be used to extract $\mathcal{C}(\text{He}) = \delta_{\text{Zem}}^A/R_3 = -1.42(4)\text{ meV fm}^{-3}$ from the $e^{-\text{He}}$ scattering data. Our calculations of $\delta_{\text{Zem}}^A$ and $R_3$ with either value of $r_p$ give $\mathcal{C}(\text{He})[r_p(e^-)] = -1.383(05)(20)\text{ meV fm}^{-3}$ and $\mathcal{C}(\text{He})[r_p(\mu^-)] = -1.388(05)(21)\text{ meV fm}^{-3}$, which both agree with Refs. [30, 31, 69].

Evidently, the nuclear-model dependence is diminished for this value, since it is proportional to the geometrical ratio $(r^3)/(2R_e^2)$. Similarly to $R_3$ discussed above, the difference between $\delta_{\text{Zem}}^A$ results obtained with the two nuclear potentials stems from the different point-proton distributions, and this largely cancels out in $\mathcal{C}$, reducing its total relative uncertainty compared to $\delta_{\text{Zem}}^A$.

Repeating the above procedures we obtain predictions for $\mu^3\text{H}$

$$\delta_{\text{Zem}}^A(\text{He})[r_p(\mu^-)] = -0.227(5)(3)\text{ meV},$$ \hspace{1cm} (13)

Ref. [31] is the arXiv version of Ref. [30], which has been updated since publication; in particular, $\delta_{\text{Zem}}^A(\text{He})$ was increased by $\sim 20\%$ with respect to the published version.

See footnote 5.
and

\[ C(\mu^3\text{H})[r_p(\mu^-)] = -0.0425(2)(6) \text{ meV fm}^{-3}. \]  

(14)

For future comparisons, using \( r_p(e^-) \) shifts \( \delta_{\text{Zem}}^A(\mu^3\text{H}) \) by \(-6\) \( \mu \text{eV} \) and \( C(\mu^3\text{H}) \) by \(+0.2 \) \( \mu \text{eV fm}^{-3} \).

Adding Eqs. (12) and (13) to Eq. (15) we obtain the total nuclear-structure TPE corrections that enter Eq. (1)

\[ \delta_{\text{TPE}}^A(\mu^3\text{He}^+) = -14.64(25)(27) \text{ meV} \]
\[ \delta_{\text{TPE}}^A(\mu^3\text{H}) = -0.703(16)(11) \text{ meV}. \]  

(16)

V. HADRONIC TPE

The last ingredient in \( \delta_{\text{TPE}} \) is the contribution from two-photon exchange with the internal degrees of freedom of the nucleons that make up the nucleus, i.e., \( \delta_{\text{TPE}}^N = \delta_{\text{Zem}}^N + \delta_{\text{pol}}^N \). Since it is dictated by the hadronic scale, about 10 times higher than the nuclear interaction, this contribution can be approximated as the sum of TPE effects with each of the individual nucleons. The various terms that contribute to \( \delta_{\text{TPE}}^N \) are estimated based on previous studies of \( \mu \text{H} \), as recently done for \( \mu \text{D} \) in Ref. [32].

Specifically, as suggested by Birse and McGovern [70], we adopt values of \( \delta_{\text{Zem}} \) and \( \delta_{\text{pol}} \) in \( \mu \text{H} \) that are combinations of results from Refs. [21, 71], as detailed below.

As Friar showed in Ref. [72], the intrinsic Zemach term of each proton contributes to \( \delta_{\text{TPE}} \) of the nucleus as an additional NS correction, not accounted for in the NS corrections detailed above.

8. We denote this term \( \delta_{\text{Zem}}^N \) and find its contribution to be proportional to the analogous term in \( \mu \text{H} \) by

\[ \delta_{\text{Zem}}^N(\mu A) = \left( \frac{Zm_r(\mu A)}{m_r(\mu H)} \right)^4 \times \delta_{\text{Zem}}(\mu H). \]  

(17)

We take \( \delta_{\text{Zem}}(\mu H) = 0.0247(13) \text{ meV} \) and obtain

\[ \delta_{\text{Zem}}^N(\mu^3\text{He}^+) = -0.487(26) \text{ meV} \]
\[ \delta_{\text{Zem}}^N(\mu^3\text{H}) = -0.0305(16) \text{ meV}. \]  

(18)

In Ref. [36], \( \delta_{\text{pol}}^N \) of \( \mu \text{D} \) was extracted from electron scattering data. Here, we resort to estimating \( \delta_{\text{pol}}^N \) by relating it to the proton polarization correction in \( \mu \text{H} \) via [34, 37, 75]

\[ \delta_{\text{pol}}^N(\mu A) = (N + Z) \left[ Zm_r(\mu A)/m_r(\mu H) \right]^3 \delta_{\text{pol}}(\mu H), \]  

(19)

assuming that the neutron polarization contribution is the same as that of the proton. Here we use \( \delta_{\text{pol}}(\mu H) = 9.3(1.1) \mu \text{eV} \). Based on current knowledge of the nucleon polarizabilities [76], we assign an additional

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8. In our notations this term appears as an NS correction to \( \delta_{\text{pol}}^{(1)} \).

9. We use the same value as in [32]. Here, \( \delta_{\text{Zem}}(\mu H) \) stands for the elastic + non-pole parts of \( \delta_{\text{TPE}}(\mu H) \), and not for the non-relativistic limit that is related to the proton’s 3rd Zemach moment (see Refs. [73, 74]).

10. \( \delta_{\text{pol}}(\mu H) = \delta_{\text{pol}}^{\text{elastic}} + \delta_{\text{pol}}^{\text{subtraction}} \). For the former we follow Ref. [39] and adopt 13.5 \( \mu \text{eV} \), which is an average of three values from Ref. [71], and for the latter we use \(-4.2(1.0) \mu \text{eV} \) from Ref [21].
20% uncertainty to the neutron polarization contribution. Another possible error in $\delta_{\text{pol}}$ arises from neglecting medium effects and nucleon-nucleon interferences in Eq. (19). These effects can be estimated by comparing the calculated $\delta_{\text{pol}}(\mu D)$ with the result evaluated in Ref. [36] from scattering data. This yields a $\sim$29% correction. Until this correction is calculated rigorously in other light muonic atoms, we estimate it to be of a similar size, multiplied by $A/2$, making it the dominant source of uncertainty in our $\delta_{\text{TPE}}$. Eventually, we obtain

$$\begin{align*}
\delta_{\text{pol}}(\mu^3\text{He}^+) &= -0.275(123) \text{ meV} \\
\delta_{\text{pol}}(\mu^3\text{H}) &= -0.034(16) \text{ meV}.
\end{align*}$$

Summing up the results in Eqs. (18) and (20) we obtain the total contribution from the nucleon degrees of freedom

$$\begin{align*}
\delta_{\text{TPE}}(\mu^3\text{He}^+) &= -0.762(125) \text{ meV} \\
\delta_{\text{TPE}}(\mu^3\text{H}) &= -0.065(16) \text{ meV}.
\end{align*}$$

In $\mu^3\text{He}^+$, $\delta_{\text{TPE}}$ is $\sim$5% of $\delta_{\text{TPE}}$, i.e., about twice the overall uncertainty in $\delta_{\text{TPE}}$. For $\mu^3\text{H}$ we obtained that $\delta_{\text{pol}}$ is $\sim$9% of $\delta_{\text{TPE}}$, which is more than three times the uncertainty in the latter. Therefore, our precision in predicting $\delta_{\text{TPE}}$ can be important not only for the determination of $R_c$ from muonic Lamb shift measurements, but also for probing $\delta_{\text{TPE}}$, if these measurements reveal discrepancies with electronic experiments that may indicate exotic contributions to $\delta_{\text{TPE}}$. A study of the Lamb shift in $\mu^3\text{H}$ will be especially sensitive to the nucleon polarizabilities, since their relative contribution is much larger in this case.

VI. SUMMARY

We have performed the first ab initio calculation of $\delta_{\text{zem}}$ and $\delta_{\text{pol}}$ for both $\mu^3\text{He}^+$ and $\mu^3\text{H}$, using state-of-the-art nuclear potentials. Many possible sources of uncertainty have been considered, yet the resulting uncertainties of a few percentcs are much lower than in previous estimates of $\delta_{\text{pol}}$ and $\delta_{\text{TPE}}$, which relied on imprecise data and simplistic models. In addition, our $\delta_{\text{pol}}$ calculations agree with previous estimates and with recent analysis of $e^{-}\text{He}$ scattering, and provide predictions towards $^3\text{H}$ measurements. They were also adapted for muonic systems by incorporating $r_p(\mu^-)$ — the proton radius measured with muons.

Ultimately, our results will allow two alternative ways of extracting a much more precise $R_c$ from a recent measurement [5, 28, 77] of the Lamb shift in $\mu^3\text{He}^+$, and from an analogous measurement we encourage to conduct in $\mu^3\text{H}$. The precision of the charge radii of $^3\text{He}$ and $^3\text{H}$ could be thus improved by factors of $\sim$5 and $\sim$50, respectively, which could have interesting implications for nuclear physics.

Finally, we estimate the hadronic contribution $\delta_{\text{TPE}}$ in these systems, and find it to be larger than our uncertainty estimates in $\delta_{\text{TPE}}$. Therefore, this combined theoretical and experimental effort may not only shed some light on the “proton radius puzzle,” but could also probe the elusive nucleon polarizabilities tightly connected to it.

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Supplementary Materials

Appendix A: error estimation

We consider many sources of uncertainty. Below we explain the origin and derivation of each uncertainty estimate.

Numerical: First we estimate the numerical accuracy of the calculations. In the EIHH method \[48, 49\], the calculations are usually repeated with the model space truncated at increasing values of the maximal hyperangular momentum \(K_{\text{max}}\), until the differences between consecutive \(K_{\text{max}}\) results become negligible. Accordingly, the numerical uncertainty can be estimated, as in \[38\], from the difference between two results obtained with different \(K_{\text{max}}\) values. However, unlike Ref. \[38\], here we encountered very slow convergence\(^{11}\), especially with the \(\chi\text{EFT}\) potential, and particularly for the \(\delta^{(2)}\) terms, which turned out to be more sensitive to the parameterization of the hyperradial grid. Consequently, the final values we provide for many terms\(^{12}\) were obtained by extrapolating the results of several calculations made with different \(K_{\text{max}}\) values. Therefore, for some of our results the numerical uncertainty was estimated from these extrapolations.

Nuclear model: Next we note the dependence of the results on the nuclear model, which is probed as in Ref. \[38\] by using the AV18/UIX and \(\chi\text{EFT}\) potentials. The final values we present are obtained by taking the mean value of the two results. As in Refs. \[35, 38\], the corresponding uncertainty is estimated as their difference divided by \(\sqrt{2}\), to account for the possibility that the “true” result lies outside the range bounded by the two calculated results.

ISB: The next source of uncertainty stems from the conservation of isospin symmetry in our calculations, i.e., we assume that the total isospin is a conserved quantity throughout the calculation. All nucleons are taken to be of equal mass, which is the average between the proton and neutron masses. The difference between the proton and the neutron is manifested only in their gyromagnetic factors and in the electromagnetic interaction included in the NN interaction. In the \(A = 3\) nuclei, most of the isospin symmetry breaking (ISB) effect can be accounted for by allowing the nuclear ground-state wave functions to include also the channel with higher total isospin value \(T = 3/2\). This, however, increases the number of basis states in each calculation and the associated computational cost rises rapidly with \(K_{\text{max}}\). It was therefore performed selectively only to estimate the uncertainty associated with performing isospin conserving calculations.

Nucleon-size corrections: Comparing the coordinate-space and momentum-space treatments of the NS corrections we conclude that higher-order corrections to the terms we obtained are expected only at \(\delta^{(1)}_{N}\). For the Zemach moments we were able to undertake a more accurate approach, from which we estimate these higher-order corrections to be \(\sim 1.46\% \ (\sim 1.33\%)\) for \(^{\mu\text{He}}\) \((\mu^{3}\text{H})\). However, for consistency we use here only the low-\(Q^2\) approximation of the nucleon electric form factor, and use the above corrections to estimate the NS-related uncertainties of the \(\delta^{(1)}\) terms.

Relativistic corrections: As explained in Section 2, relativistic corrections were included only for the leading electric dipole contribution \(\delta^{(0)}_{D1}\). Their sum turned out to be \(2.0\% \ (2.1\%)\) of the non-relativistic value in \(^{4}\text{He}\) \((^{3}\text{H})\). We therefore estimated the uncertainty due to uncalculated relativistic corrections of the other contributions to be of that relative size. We would like to point out two aspects of the elastic (Zemach) term: (i) Comparing the non-relativistic calculation of \(\delta^{A}_{\text{zem}}\) of \(\mu\text{D}\) in Ref. \[35\] with the relativistic treatment in Ref. \[36\] reveals a discrepancy of the same order as the uncertainty estimate given above. (ii) We calculate \(\delta^{A}_{\text{zem}}\) according to the definition that connects it to the nuclear Zemach moments. Therefore, no relativistic corrections are needed in the comparison we make with similar results in the literature. However, when our value for \(C\) is used to approximate the full elastic part of \(\delta^{A}_{\text{rep}}\) in Eq. (1), the missing relativistic corrections should be accounted for. In this context, the total relative uncertainty of \(C\) should be increased to \(2.5\%\).

Coulomb corrections: Following Ref. \[37\], we estimate higher-order Coulomb corrections to be \(\sim 6\%\) of \(\delta^{(2)}\).

Multipole expansion: As in Ref. \[38\], our multipole expansion is truncated at \(\delta^{(2)}\). Based on our results we conservatively estimate 2% uncertainty in \(\delta^{A}_{\text{pol}}\) due to this truncation.

\(^{11}\) This may be due to the larger radii of the \(A = 3\) nuclei compared with \(^{4}\text{He}\), and was indeed slightly worse for \(^{3}\text{He}\) than for \(^{3}\text{H}\).

\(^{12}\) Depending on the nucleus and the nuclear potential, some of the following terms were obtained with the aid of extrapolations: BE, \(\alpha_{E}\), the individual \(\delta^{(2)}\) terms (including \(\delta^{(2)}_{N,S}, \delta^{(2)}_{M}\)), and the sum of all other \(\delta^{(0)}\) terms.
**Zα expansion:** Except for the logarithmically enhanced Coulomb distortion contribution, we include in our calculation of δₚₒˡ all terms of order (Zα)⁵. Since (Zα) is small for these systems, the missing contribution from all the higher-order terms can be approximated by the first unaccounted-for term in the series, (Zα)⁶, which is naturally estimated to be (Zα) ≃ 1.46% (0.73%) of the size of δₚₒˡ in ³He (³H).

**Magnetic MEC contribution:** The magnetic dipole term δ(0)ₘ is calculated using the impulse approximation (IA) operator, and is therefore missing significant corrections, mainly due to meson-exchange currents (MECs). The same IA operator was also used to calculate the magnetic moment ˆµₙ in the nuclear ground state. The results, presented in Table I, show a deviation of the IA ˆµₙ calculated with the AV18/UIX (χEFT) potential from the very precise experimental values by 23% (21%) for ³He and 15% (13%) for ³H. The same relative errors were therefore assumed also for the small IA value obtained for δ(0)ₘ.

The total uncertainties were obtained as a quadrature sum of all the above, where the last five sources do not affect the Zemach terms. The values we thus obtained for the individual and total relative uncertainties estimated for δₚₒˡ, δₚₑₒˡ, and δₜₚₑ in ³He⁺ and ³H are given in Table S1 below. We remind the reader that δₜₚₑ ≡ δₚₑₒˡ + δₚₒˡ can be obtained directly from our results, by summing all terms in δₚₒˡ except for the Zemach terms, due to their cancellation.

Table S1. Estimated relative uncertainties, in percents, assigned to the calculated nuclear TPE corrections to the 2S-2P Lamb shift in µ³He⁺ and µ³H. The presented values are rounded. The total uncertainties are obtained from a quadrature sum.

| Error type          | µ³He⁺ | µ³H  |
|---------------------|------|------|
|                     | δₚₒˡ | δₚₑₒˡ| δₜₚₑ | δₚₒˡ | δₚₑₒˡ| δₜₚₑ |
| Numerical           | 0.4  | 0.1  | 0.1  | 0.1  | 0.0  | 0.1  |
| Nuclear model       | 1.5  | 1.8  | 1.7  | 2.2  | 2.3  | 2.2  |
| ISB                 | 2.0  | 0.2  | 0.5  | 0.9  | 0.2  | 0.6  |
| Nucleon size        | 1.6  | 1.5  | 0.6  | 0.6  | 1.3  | 0.0  |
| Relativistic        | 0.6  | -    | 1.5  | 1.4  | -    | 0.3  |
| Coulomb             | 1.2  | -    | 0.3  | 0.3  | -    | 0.2  |
| Multipole expansion | 2.0  | -    | 0.6  | 2.0  | -    | 1.4  |
| Higher Zα           | 1.5  | -    | 0.4  | 0.7  | -    | 0.5  |
| Magnetic MEC        | 0.4  | -    | 0.1  | 0.3  | -    | 0.2  |
| Total               | 4.1% | 2.3% | 2.5% | 3.6% | 2.7% | 2.7% |

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13 See Refs. [58, 59] and Refs. therein.
Appendix B: List of individual contributions to the nuclear polarization energy correction

Table S2. Nuclear structure corrections to the 2S-2P Lamb shift $\Delta E$ [meV] in $\mu^3$He$^+$ and $\mu^3$H, obtained with the AV18/UIX and $\chi$EFT nuclear potentials. The brackets show only the numerical error in the presented precision. See text for details regarding the individual terms.

|                | $\mu^3$He$^+$ | $\mu^3$H |
|----------------|---------------|---------|
| $\delta^{(0)}$ | $\delta^{(0)}_{L}$ | $\delta^{(0)}_{T}$ | $\delta^{(0)}_{P}$ | $\delta^{(0)}_{S}$ |
| AV18/UIX       | -6.479(06)    | -0.103(00) | 1.000(01) | -5.346(05) |
| $\chi$EFT      | 0.232(00)     | 0.240(00)  | 1.020(03) | 0.047(00) |
| sum            | 0.081(02)     | 0.047(00)  | 0.0101(3) | 0.0058(00) |

| $\delta^{(1)}$ | $\delta^{(1)}_{R3}$ | $\delta^{(1)}_{Z1}$ |
|----------------|---------------------|---------------------|
| $\delta^{(2)}$ | $\delta^{(2)}_{R2}$ | $\delta^{(2)}_{Q}$  | $\delta^{(2)}_{D1,D3}$ |
| AV18/UIX       | 8.100(10)           | 1.015(01)           | -0.841(00)           |
| $\chi$EFT      | 8.327(3)            | 1.038(00)           | -0.862(00)           |
| sum            | 1.000(01)           | 0.1778(00)          | -0.0783(1)           |

| $\delta_{NS}$ | $\delta_{NS}$ |
|----------------|---------------|
| $\delta_{A}$  | $\delta_{A}$ |
| AV18/UIX       | -4.114(17)   | -10.356(10) |
| $\chi$EFT      | -4.201(8)    | -10.618(3) |
| $\delta_{A}$   | -4.470(14)   | -14.470(14) |

The brackets show only the numerical error in the presented precision. See text for details regarding the individual terms.