The proton structure in and out of muonic hydrogen

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Abstract
Laser spectroscopy of muonic atoms has been recently used to probe properties of light nuclei with unprecedented precision. We introduce nuclear effects in hydrogen-like atoms, nucleon structure quantities (form factors, structure functions, polarizabilities) and their effects in the Lamb shift and hyperfine splitting (HFS) of muonic hydrogen (µH). Updated theory predictions for the Lamb shift and HFS in µH are presented. We review the challenges of the ongoing effort to measure the ground-state HFS in µH and its impact on our understanding of the nucleon spin structure. To narrow down this search, we present a novel theory prediction obtained by scaling the measured HFS in hydrogen leveraging radiative corrections. We also summarize recent developments in the spectroscopy of simple atomic and molecular systems and emphasize how they allow for precise determinations of fundamental constants, bound-state QED tests and New Physics searches.
1. Introduction

μH — a hydrogen with the electron replaced by a muon — has an enhanced sensitivity to the proton structure and the short-range effects in general. The enhancement factor, as compared to H, is of order \( \left( \frac{m_\mu}{m_e} \right)^3 \approx 10^7 \), making μH a neat laboratory for studies of the proton structure. The same applies to other muonic atoms, where the neutron structure can be explored, along with the structure of the atomic nucleus as a whole.

The last decade has witnessed a remarkable breakthrough in the laser spectroscopy of muonic atoms, starting from the long-awaited observation of the 2S-2P transition in μH by the CREMA Collaboration (1, 2). This transition appeared to be quite far from the predicted value, which made it very difficult to find, and very intriguing when found. It inferred a proton charge radius, \( r_p \), which was spectacularly \((7\sigma)\) smaller than the state-of-the-art value of that time (see CODATA ’10 (3) in Fig. 1). The CODATA value comprised decades of \( r_p \) determinations using the traditional techniques: ep scattering and H spectroscopy.

This resounding discrepancy, known as the proton-radius puzzle, stirred a wealth of activity at the intersection of nuclear, particle, and atomic physics, reaching out to physics beyond the Standard Model (see Refs. 4–7, for recent reviews). The subsequent measurement of the μD Lamb shift (8) revealed a similar discrepancy for the deuteron charge radius, \( r_d \), see Fig. 2. The two discrepancies are, in fact, related by the H-D isotopic shift measurement of the 1S-2S transition (9), which constrains the difference, \( r_d^2 - r_p^2 \). They are sometimes commonly referred to as the “\( Z = 1 \) radius puzzle”, emphasizing that no such discrepancy has been found in muonic helium (10). Using the theory updates of Refs. 11–13 and 14, the \( r_p \) value obtained from μD via the isotopic shift is in agreement with the value extracted directly from μH on the permille level.

Today, more than a decade after the radius-puzzle installment, there is some consensus, adopted also by the CODATA group (15), that the μH value is, not only an order-of-

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**H, D**: Hydrogen, deuterium.

**μH, μD**: Muonic hydrogen, muonic deuterium.

**ep, μp**: Electron-proton, muon-proton scattering.
Selection of recent proton charge radius determinations. For references, see respectively (from top to bottom): CODATA (15, 16, 3), muonic atoms (11, 2, 1), H spectroscopy (17–21, 16), ep scattering (22–27), dispersive analysis of ep scattering (28–31). The vertical band is aligned with the $\mu H$ '13 value (2).

Proton charge radius: definition via slope of the electric Sachs form factor, $r_p = \sqrt{-6G_E}(0)$. 

magnitude more precise, but also, more accurate. The problem with the previous extractions may simply lie in unaccounted systematic uncertainties — a rather boring solution of the puzzle; at least in comparison with most of the other proposals. This view is corroborated by some of the recent (re-)measurements using H. With exception of the H(1S-3S) transition measurement by the Paris group (20), the other four new measurements in H yielded smaller radii than the CODATA '10: three of them in agreement with the muonic results (18, 19, 21), a very recent one of the H(2S−8D) (17) though in some tension, that calls for the need of further experimental determinations.

On the side of ep scattering, the recent PRad experiment (22) has found the smaller value of $r_p$, in agreement with $\mu H$, confirming several analysis of scattering data that agree with the muonic result (23, 24, 28–31). The initial-state radiation experiment at MAMI has a larger uncertainty, thus, does not allow to discriminate between the small and large radius scenarios at the moment (32).

Complementing the picture with these latest results diffuses the discrepancy quite considerably, see Fig. 1. Nonetheless, the jury is still out and a new round of experiments is underway, including first measurements from $\mu p$ scattering by MUSE (33) and AMBER collaborations (34), improved ep scattering measurements from PRAD-II (35) and the PRES Collaboration at MAMI, as well as spectroscopy measurements of H in Rydberg states (36), He$^+$(1S-2S) (37, 38) and simple molecules such as HD$^+$, H$_2^+$ and H$_2$ (see Sec. 5.3).

It is also interesting to look beyond the puzzle. What else can be learned from the muonic atoms, in conjunction with atomic spectroscopy and scattering experiments? Likewise, how the improved $r_p$, and other structure information extracted from muonic atoms,
will impact the precision of other experiments, and, more generally, contribute to a better understanding of the Standard Model and beyond?

For example, the proton radius from $\mu$H, in combination with the $1S-2S$ transition in H, leads to the most precise determination of the Rydberg constant $R_\infty$. In combination with the H-D isotopic shift, it leads to the most precise determination of the deuteron radius. The latter, combined with the measured Lamb shift in $\mu$D, provides a stringent test for the theory of the deuteron structure, viz., the nucleon-nucleon interaction. The proton radius combined with spectroscopy of H, D, HD$^+$ and other simple systems, can be used to perform precision tests of bound-state QED for few-body systems, impacting the precision of various fundamental quantities. While at the moment HD$^+$ can barely favor the muonic results (39), its potential is enormous. On the scattering side, the precise value of $r_p$ allows for a better determination of the proton electric form factor $G_{Ep}(Q^2)$. These are some of the “ins and outs” that will be addressed in this article. Obviously, with increasing precision one becomes sensitive to certain scenarios beyond the Standard Model, beyond the ones proposed as explanation of the puzzle in the first place, e.g., Refs. 40–43.

Another topic of our interest here concerns the ongoing efforts to measure the ground-state hfs in $\mu$H. The CREMA Collaboration is aiming at the measurement with 1 ppm relative accuracy by means of pulsed laser spectroscopy. In parallel, two other collaborations, at J-PARC (46) and RIKEN-RAL (47–51), are developing measurements of this transition using different techniques. The hfs resonance is two orders of magnitude narrower than the $2S-2P$ line width, hence, difficult to find. We shall examine the prospects for an accurate prediction of this transition, which will help to guide the upcoming searches, and discuss what can be learned when this transition is found.

This paper is organised in the following way. Section 2 provides a brief introduction into the nuclear-structure corrections, with emphasis on radiative corrections important for $\mu$H. Section 3 is devoted to evaluations of the proton-polarizability contribution. Section 4 provides updated theory predictions for the $\mu$H Lamb shift and the hfs in H and $\mu$H. In

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**hfs**: Hyperfine splitting.  
**$\mu$H hfs experiments**: Ongoing efforts to measure the $1S$ hfs in $\mu$H with 1 ppm accuracy.
Section 5, we elaborate more on the central role of HD+ spectroscopy and H to extend the impact of the proton radius measurement to other precision quantities and possible New Physics searches. Section 6 presents a list of future prospects. Note that we are using natural units ($\hbar = c = 1$), unless specified otherwise.

2. Brief introduction to nuclear effects in hydrogen-like atoms

Muonic atoms have a distinctly small Bohr radius, and therefore a larger sensitivity to nuclear structure, and short-range effects in general. While the finite-size contribution is increased by the aforementioned factor of $10^7$, relative to normal atoms, the QED effects contributing to the $2S-2P$ splitting increase only by a factor of 50, promoting the finite-size contribution to be the second largest contribution, trumped only by the one-loop eVP, shown in Fig. 3(a) and discussed in Sec. 2.1 of the Supplement. The literature accounting for these effects is very extensive, see, e.g., Refs. 52–56. And nevertheless, the work on accurate calculations of these effects will continue in the foreseeable future, as the ongoing experiments bode new leaps in precision. Important for this program is the progress on the nuclear side, since many of the corrections require the input of nuclear and nucleon form factors and structure functions. In this section, and Sec. 3, we briefly describe how these ingredients are entering the atomic calculations; some numerical results for $\mu H$ are discussed in Sec. 4.

The starting point is, of course, the Coulomb problem solved by using either the Dirac or Schrödinger equation (57). A short recap of the quantum-mechanical Coulomb problem is given in Sec. 1 of the Supplement. It assumes a pointlike nucleus with the electric charge $Ze$, whereas the effects beyond this approximation come as perturbative corrections to the Lamb shift, fine and hyperfine structure. The perturbation series is organized in powers of the fine-structure constant $\alpha = e^2/4\pi$, and mass ratios. Among the nuclear-structure effects, we distinguish (i) the finite-size effects, which come from the electromagnetic distributions in the nucleus [e.g., Fig. 3 (b-d)], and (ii) the polarizability effects [Fig. 4 (a)], caused by deformations of the distributions within the atom. The former can be entirely described by the elastic form factors, such as $G_E(Q^2)$ and $G_M(Q^2)$ in case of a spin-1/2 nucleus (e.g., the proton), whereas the latter require a more complicated input, viz., structure functions. The two types of effects are also treated quite differently, as will be seen in the following derivation of the leading and next-to-leading nuclear contributions.

Bohr radius: $a_B = (Z\alpha m_e)^{-1}$, with reduced mass $m_r = mM / (m + M)$, where $m$ and $M$ are the lepton and nucleus masses.

eVP, $\mu$VP, hVP: Vacuum polarization due to electrons, muons, hadrons.

![Figure 3](image-url)

Major corrections discussed in the text. The cyan blobs represent the finite-size effects, thin and thick lines the muon and proton, respectively.
2.1. Finite-size effects

Let us start by discussing the finite-size effects, that can be described through the charge, Friar and Zemach radii, as well as higher moments of the electromagnetic distributions.

2.1.1. Lamb shift. The main nuclear effect in the Lamb shift comes from the nuclear charge distribution $\rho_E(r)$, which, in momentum space, is described by an electric form factor (eFF) $G_E(Q^2)$, function of the photon virtuality, $Q^2 = q^2 - q_0^2$. The corresponding potential is [see Fig. 3(b)]:

$$V_{\text{eFF}}(q) = \frac{4\pi Z\alpha}{q^2} [G_E(q^2) - 1] = \frac{1}{\pi} \int_{t_0}^{\infty} \frac{dt}{t} \text{Im} G_E(t) \frac{4\pi Z\alpha}{q^2 + t},$$

neglecting the relativistic effects, such as the dependence on the energy transfer $q_0$ (retardation) and recoil corrections, which can be treated within the Breit-potential formalism, cf. (58, Ch. IX, §83). The two forms of the potential in Eq. 1 are related by the once-subtracted dispersion relation:

$$G_E(Q^2) = 1 - \frac{Q^2}{\pi} \int_{t_0}^{\infty} \frac{dt}{t} \frac{\text{Im} G_E(t)}{t + Q^2 - t_0^2},$$

where the integration is done over the timelike region, where the form factor develops a discontinuity associated with particle production, with $t_0$ being the lowest threshold. For the proton, for instance, the leading discontinuity is associated with two-pion production, i.e., $t_0 = 4m^2$.

In principle, the absorptive part of the form factor, $\text{Im} G_E(t)$, is known empirically (see, e.g., Refs. 28–31 for the proton). However, here we use the dispersive representation simply as a convenient analytical tool. In coordinate space, where the Coulomb potential is given by $-Z\alpha/r$, the form-factor correction takes the following form,

$$V_{\text{eFF}}(r) = \frac{Z\alpha}{\pi} \int_{t_0}^{\infty} \frac{dt}{t} \text{Im} G_E(t) \frac{1}{r} e^{-r/\sqrt{t}},$$

which, in fact, is the Yukawa potential with the dispersed mass given by $\sqrt{t}$. As a result, the 1st-order perturbation-theory contribution to the classic $(2S - 2P)$ Lamb shift is given by:

$$E^{(\text{eFF})}_{2S-2P} = \langle 2S|V_{\text{eFF}}|2S \rangle - \langle 2P|V_{\text{eFF}}|2P \rangle = \frac{(Z\alpha)^4 m_e^3}{2\pi} \int_{t_0}^{\infty} dt \frac{\text{Im} G_E(t)}{(\sqrt{t} + Z\alpha m_e)^2}.$$

Since $Z\alpha m_e \ll \sqrt{t_0}$, the denominator can be expanded (assuming the atomic Bohr radius is much larger than the nuclear size), yielding:

$$E^{(\text{eFF})}_{2S-2P} = \frac{(Z\alpha)^4 m_e^3}{12} \sum_{k=2}^{\infty} \frac{(-Z\alpha m_e)^{k-2}}{(k-2)!} \left\{ r_K^k \right\} = \frac{(Z\alpha)^4 m_e^3}{12} \left\{ r^2_E - Z\alpha m_e \langle r^3_L \rangle + \ldots \right\},$$

where $\left\{ r_K^k \right\}$ is the $k^{th}$ moment of the charge distribution $\rho_E(r)$:

$$\langle r_K^k \rangle = 4\pi \int_0^{\infty} dr r^{2+k} \rho_E(r) = \frac{(k+1)!}{\pi} \int_{t_0}^{\infty} dt \frac{\text{Im} G_E(t)}{t^{1+k/2}}.$$
compute the next term of order \( (Z\alpha)^5 \) correctly, we ought to take this correction to the 2nd-order perturbation theory:

\[
E_{2S-2P}^{(e\text{FF})(\text{eFF})} = \frac{\int_{n=2} |\langle 2S|V_{e\text{FF}}|nS\rangle|^2 - |\langle 2P|V_{e\text{FF}}|nP\rangle|^2}{E_2 - E_n} \]

\[
\equiv \frac{2(Z\alpha)^5 m_e^4}{\pi} \int_0^\infty \frac{dQ}{Q^4} \left[ G_E(Q^2) - 1 \right]^2 = \frac{(Z\alpha)^5 m_e^4}{12} \left( \langle r_E^3 \rangle - \frac{1}{2} \langle r_E^3 \rangle_{(2)} \right), \quad 7.
\]

where we only kept terms of order \( (Z\alpha)^5 \) and introduced the 3rd Zemach moment (59):

\[
\langle r_E^3 \rangle_{(2)} = \frac{48}{\pi} \int_0^\infty \frac{dQ}{Q^4} \left[ G_E^2(Q^2) - 1 + \frac{1}{4} \langle r_E^2 \rangle Q^2 \right]. \quad 8.
\]

with the corresponding radius called the Friar radius. One sees that the 2nd-order contribution essentially replaces the third radius, appearing in Eq. 5, with the Friar-radius term. To order \( (Z\alpha)^5 \), the finite-size correction is then given by

\[
E_{2S-2P}^{fs} = \frac{(Z\alpha)^5 m_e^3}{12} \langle r_E^2 \rangle - \frac{(Z\alpha)^5 m_e^4}{24} \langle r_E^3 \rangle_{(2)}. \quad 9.
\]

Similarly, to compute the complete order-\( (Z\alpha)^6 \) correction, one needs to take this potential to the 3rd-order, and so forth. The first corrections that affect \( P \)-levels begin at order \( (Z\alpha)^6 \). Thus, up to this order, the entire effect can be deduced from a \( \delta(r) \)-function potential, which provides an easy generalisation for the \( nS \)-level shift:

\[
E_{nS}^{fs} = \frac{2\pi}{\gamma} Z\alpha \left( \langle r_E^2 \rangle - \frac{1}{2} Z\alpha m r \langle r_E^3 \rangle_{(2)} \right) \phi_{nS,0}^2, \quad 10.
\]

with \( \phi_{nS,0}^2 \) the wave function at the origin. The Friar-radius contribution is obviously playing a more significant role in \( \mu \text{H} \) than in \( \text{H} \), and was an initial suspect to resolve the proton-radius puzzle (60). However, in that scenario, the Friar radius was so large that the expansion in radii would be invalid (61, 62). The present consensus is that this contribution is at least an order-of-magnitude smaller than what is required for the explanation of the puzzle. Furthermore, there are relativistic corrections, which can be treated within the Breit-potential formalism, or alternatively, by considering the two-photon exchange, as will be seen below. Also important are some radiative corrections, which come from combining the finite-size and QED effects. In muonic atoms, the eVP plays an especially prominent role, and produces sizeable radiative corrections to the finite-size effects shown in Fig. 3 (c) and (d), considered in Sec. 2.3.

### 2.1.2. Hyperfine splitting

Assuming a spin-1/2 nucleus, the hfs arises from the magnetisation properties of the nucleus described by the magnetic form factor \( (\text{mFF}) G_M(Q^2) \). For the \( S \)-levels, the corresponding potential is given by (omitting recoil corrections):

\[
V_{nS}^{\text{mFF}}(q) = \frac{4\pi Z\alpha}{3m_M} \left[ F(F+1) - \frac{3}{2} \right] G_M(q^2) = \frac{4Z\alpha}{3m_M} \left[ F(F+1) - \frac{3}{2} \right] \int_{t_0}^\infty dt \frac{\text{Im} G_M(t)}{q^2 + t}, \quad 11.
\]

where \( F = 0 \) or 1 is the total spin, \( \kappa_N \) the anomalous magnetic moment of the nucleus; \( G_M(0) = 1 + \kappa_N \) is the value of the magnetic moment in units of \( Ze/2M \). The corresponding coordinate-space potential is directly proportional to the magnetization density \( \rho_M(r) \).

\[
\text{The Friar radius:} \quad r_{\text{Friar}} = \sqrt{\langle r_E^3 \rangle_{(2)}}
\]

\[
\text{Wave function at the origin:} \quad \phi_{nS,0}^2 = 1/(\pi a_\text{H}^3 n^3)
\]
Details on the charge and magnetization densities, and the coordinate-space potentials are given in Sec. 2 of the Supplement.

The 1st-order contribution, yields the following hfs interval of the nS-level:

$$E_{nS-hfs}^{(mFF)} = \left(1 - 2Z\alpha m_r(r_M)\right)\frac{E_F}{n^3} + O[(Z\alpha)^6].$$

where $E_F$ is the Fermi energy, and $(r_M) = 4\pi \int_0^\infty dr r^3 \rho_M(r)$ is the linear magnetic radius. At the 2nd order, the interference with the eFF potential of Eq. 1, gives:

$$E_{nS-hfs}^{(mFF)(eFF)} = Z\alpha m_r \left( (r_M) - r_Z \right) \frac{E_F}{n^3} + O[(Z\alpha)^6],$$

thus cancelling the linear magnetic radius term from the 1st order, and installing instead the Zemach radius:

$$r_Z = \frac{4}{\pi} \int_0^\infty dQ \frac{4}{Q^2} \left[ \frac{G_E(Q^2)G_M(Q^2)}{1 + \kappa N} - 1 \right].$$

The Fermi-energy contribution is not a finite-size effect, as it is already present for a pointlike nucleus. The leading finite-size effect in the hfs is therefore of order $(Z\alpha)^5$,

$$E_{nS-hfs}^{\ell,s} = -(2Z\alpha m_r/n^3)E_F r_Z.$$

At this order, also the polarizability corrections begin to appear. We consider them next.

### 2.2. Two-photon exchange and polarizability effects

The Fermi energy:

$$E_F = \frac{8(Z\alpha)^4 m_r^2 (1 + \kappa_N)}{3m_M}$$

Thus far, we considered effects which stem from the one-photon exchange and its iterations, such that the nucleus stays intact and in its ground state. There are also effects coming from nuclear excitations, which can only be assessed through a 2γ exchange, see Fig. 4(a). This description goes beyond the elastic form factors and involves instead the polarizabilities and inelastic structure functions, as will be seen in what follows.

The 2γ exchange in Fig. 4(a) introduces, in general, a correction $V_{2\gamma}(p' - p; p', p)$ which depends on the relative momenta of the initial and final state, $p$ and $p'$, as well as the momentum transfer $q = p' - p$. These are four-momenta, but the energy effects can safely be neglected, since they are suppressed by $(Z\alpha)^2 m_r$. The dependence on $|p| = |p'|$ is suppressed by $Zam_r$ and will, to leading order, be neglected too. The dependence on $|q|$ is a bit more
It remains now to calculate $V_{2\gamma}$ expressed everything in terms of integrals of the structure functions, the dispersion relations for the forward Compton amplitude, see Fig. 4(c), which allows one to the larger contribution, of order $1/(m + M)^2$:

$$V_{2\gamma}(t) = \frac{1}{\pi} \int_0^\infty dt \frac{\text{Im} V_{2\gamma}(t')}{t' - t - i0^+} = V_{2\gamma}(t = 0) + \frac{t}{\pi} \int_0^\infty dt' \frac{\text{Im} V_{2\gamma}(t')}{t'(t' - t - i0^+)},$$

where in the second equation we have a once-subtracted relation, thus introducing the forward scattering amplitude, $V_{2\gamma}(t = 0)$. The remainder with non-vanishing momentum transfer is referred to as the off-forward amplitude.

The absorptive part, $\text{Im} V_{2\gamma}(t)$, corresponds with the discontinuity across the $t$-channel cut, which starts at 0, because the photons are massless. Because of this, the expansion in $t$ is non-analytic. When calculating the level shifts in perturbation theory, this non-analyticity translates into $\log Z\alpha$ contributions.

Let us see this for the Lamb shift, where we can make use of the arguments leading to Eq. 4 and arrive at:

$$E^{(2\gamma)}_{2S-2P} = \frac{(Z\alpha_m)^3}{8\pi^2} \int_0^\infty dt \frac{t \text{Im} V_{2\gamma}(t)}{(\sqrt{t} + Z\alpha_m)^4} \tag{17a}$$

$$= V_{2\gamma}(0) \phi_{2S}(0) + \frac{(Z\alpha_m)^3}{8\pi^2} \int_0^\infty dt \left[ \frac{t}{(\sqrt{t} + Z\alpha_m)^4} - \frac{1}{t} \right] \text{Im} V_{2\gamma}(t). \tag{17b}$$

Let us focus on the leading polarizability effect, coming from the electric $\alpha_{E1}$ and magnetic $\beta_{M1}$ dipole polarizabilities of the nucleus. Knowing how they enter the Compton scattering amplitude, we can obtain their contribution to $\text{Im} V_{2\gamma}(t)$. Note that our consideration of the $2\gamma$ cut in Fig. 4(b) involves only the real Compton scattering and static polarizabilities. The expression is rather lengthy (63) and we only quote here the polarizability potential in the well-known long-range and the singular short-range limit:

$$V_{2\gamma}(r) = \frac{1}{4\pi^2 r} \int_0^\infty dt \text{Im} V_{2\gamma}(t) e^{-r\sqrt{t}} = \frac{\alpha \alpha_{E1}}{2r^3} + \frac{\alpha (11\alpha_{E1} + 5\beta_{M1})}{4\pi mr^3} + O(1/r^6). \tag{18a}$$

$$r \to 0 \quad am \log(mr) \quad (\alpha_{E1} - \beta_{M1}) + O(1/r^3). \tag{18b}$$

Note that the prefactor of $\alpha$ is coming from the lepton line, whereas the polarizabilities contain $Z^2\alpha$, hence in total the order is $(Z\alpha)^2$ as expected. The entire potential is negative-definite (attractive), provided $\alpha_{E1} > \beta_{M1}$, and assuming the electric polarizability is a positive-definite quantity. This potential, however, is not very useful to compute the contribution to the $S$-states, because of the singular short-range behavior. Anticipating that, we have introduced the subtracted dispersion relation in Eq. 16, leading to Eq. 17b. The integration over $t$ is now convergent, the short-range contribution regularized, and, for the leading-$Z\alpha$ contribution to the $nS$-shift, we obtain:

$$E^{(2\gamma)}_{nS} = \{V_{2\gamma}(0) + 4\alpha(Z\alpha) \alpha_{E1} \log[2n(Z\alpha)^{-1}] + O[(Z\alpha)^3]\} \phi_{nS}^2(0). \tag{19}$$

It remains now to calculate $V_{2\gamma}(0)$, i.e., the forward $2\gamma$ exchange, as it apparently gives the larger contribution, of order $(Z\alpha)^3$. For this, one can make use of the $s$-channel dispersion relations for the forward Compton amplitude, see Fig. 4(c), which allows one to express everything in terms of integrals of the structure functions, $F_{1,2}(x, Q^2)$, measured
in inclusive electron scattering. Unfortunately, one of these dispersion relations requires a subtraction too, which precludes the use of a purely data-driven approach. Still, most of the existing calculations are based on the data-driven approach, in conjunction with some model-building of the subtraction function. Alternatively, one can calculate the entire \((Z\alpha)^5\) contribution using \(\chi PT\) or lattice QCD. More details on evaluations of the forward \(2\gamma\)-exchange contribution can found in Sec. 3.

Similar consideration can be done for the hfs. There are two important differences: the contribution of order \((Z\alpha)^6\log Z\alpha\) is absent, and the order \((Z\alpha)^5\) — the forward \(2\gamma\)-exchange contribution — can be expressed in terms of the spin structure functions without a subtraction, see Sec. 3 for details. There is an interesting order-(\(Z\alpha\))^6 contribution coming from the neutral-pion exchange, which couples to the lepton through the chiral anomaly (64–67). However, it is not very relevant at the current level of precision. It will become, perhaps, once the \(\mu H 1S\) hfs is measured.

### 2.3. Radiative corrections

The largest corrections in muonic atoms involve the eVP, which also produces radiative corrections to the finite-size effects via the mechanisms of Figs. 3 (c) and (d). They are respectively referred to as VP1 and VP2.

#### 2.3.1. VP2 correction [Fig. 3(d)].

The diagram appears from the interference of the finite-size correction \(V_{\text{eFF}}\), Fig. 3(b), with the Uehling potential, Fig. 3(a), at the 2\(^\text{nd}\)-order perturbation theory. To avoid lengthy considerations, we cast the finite-size effects into a \(\delta(r)\)-function potential, as remarked above (valid for contributions that only influence the \(S\)-levels). The eVP effect then amounts to correcting the wave function at the origin, appearing in Eq. 10, as follows:

\[
\phi_{n,S}^2(0) \to \phi_{n,S}^2(0) \left[ 1 + \frac{\alpha}{\pi} C_1(nS) \right],
\]

where \(C_1(nS)\) is known analytically for the case of one-loop eVP, see (68, Eq. B3). This is the universal eVP correction to any \(\delta\)-function potential, including the forward \(2\gamma\)-exchange correction considered in Sec. 3.

#### 2.3.2. VP1 correction to the Lamb shift [Fig. 3(c)].

This correction corresponds to the following potential,

\[
V_{\text{eFF}, \text{VP1}}(q) = -\frac{4\pi Z\alpha}{q^2} \left[ G_E(q^2) - 1 \right] \Pi(q^2),
\]

where \(\Pi(Q^2)\) is the scalar part of the vacuum polarization. Using the dispersive representation, the correction to Eq. 4 reads:

\[
E_{2S-2P}^{\text{VP1}} = \frac{(Z\alpha)^4 m_e^3}{2\pi} \left[ \int_{t_0}^{\infty} dt \frac{\text{Im} G_E(t) \text{Re} \Pi(-t)}{(\sqrt{t} + Z\alpha m_e)^4} + \int_{4m_e^2}^{\infty} dt \frac{[\text{Re} G_E(-t) - 1] \text{Im} \Pi(t)}{(\sqrt{t} + Z\alpha m_e)^4} \right] + \ldots
\]

\[
= \frac{(Z\alpha)^4 m_e^3}{2\pi} \left[ \int_{4m_e^2}^{\infty} \frac{[\text{Re} G_E(-t) - 1] \text{Im} \Pi(t)}{(\sqrt{t} + Z\alpha m_e)^4} \right] + O\left(\frac{Z\alpha m_e}{\sqrt{t_0}}\right).
\]
Within the indicated approximations this correction affects only the charge-radius contribution:

\[ E_{2S-2P}^{\text{VP}} = \frac{1}{12}(Z\alpha)^4 m_e^3 \left( (1 + \delta_{2S-2P}^{\text{VP1}}) \left( \frac{r_E^3}{2} \right) - \frac{1}{2} Z \alpha m_e \frac{r_E^3}{2} \right) \]

\[ \delta_{2S-2P}^{\text{VP1}} = \frac{1}{\pi} \int_{-\infty}^{\infty} dt \left[ \frac{1}{(\sqrt{t} + Z \alpha m_e)^2} - \frac{1}{t^2} \right] \text{Im}\Pi(t). \]

Substituting the one-loop expression for the eVP (i.e., \( \text{Im}\Pi^{(1)}(t) \) displayed in Eq. 14 of the Supplement), we obtain:

\[ \delta_{2S-2P}^{\text{VP1}(1)} = \frac{\alpha}{6\pi(1 - \kappa^2)^2} \left[ \kappa(4\kappa^2 - 7) + \frac{4\kappa^4 - 10\kappa^2 + 9}{\sqrt{1 - \kappa^2}} \arccos\kappa \right], \quad \text{with} \quad \kappa = \frac{Z \alpha m_e}{2m_e}. \]

For \( \mu \), \( \delta_{2S-2P}^{\text{VP1}(1)} = 2.155 \times 10^{-3} \). Note that this correction affects both the \( S \) - and \( P \)-levels.

### 2.3.3. VP1 correction to hfs [Fig. 3(c)]

The eVP radiative corrections to the hfs are treated similarly. In this case the potential corresponding to the diagram of Fig. 3(c) is:

\[ V_{\text{VP1}}^{\text{hfs}}(q) = \frac{8\pi Z\alpha}{3m_M} G_M(q^2) \Pi(q^2). \]

Going through the same steps as in Eq. 22, one finds the following effect on the ground-state hfs:

\[ E_{1S-\text{hfs}}^{\text{VP1}} = \frac{8(Z\alpha)^4 m_e^3}{3\pi m_M} \int_{4m_e^2}^{\infty} dt \frac{\text{Re}\Pi(t)}{s(t)} \frac{1}{(\sqrt{t} + Z \alpha m_e)^2 - \frac{1}{t}} \]

\[ = -4Z \alpha m_e \int_{t_0}^{\infty} dt \frac{\text{Im}\Pi(t)}{t^{3/2}} \text{Re}\Pi(t) + O(\left(Z \alpha m_e^2\right)^2). \]

The first term is not a finite-size correction as it only affects the Fermi-energy term, albeit differently for each \( nl \). For the ground state, its effect is \( E_F \left( 1 + \delta_{2S-\text{hfs}}^{\text{VP1}} \right) \), where the one-loop eVP gives:

\[ \delta_{1S-\text{hfs}}^{\text{VP1}} = \frac{1}{\pi} \int_{4m_e^2}^{\infty} dt \left[ \frac{1}{(\sqrt{t} + Z \alpha m_e)^2} - \frac{1}{t} \right] \text{Im}\Pi^{(1)}(t) \]

\[ = \frac{\alpha}{3\pi\kappa_1^3} \left[ 2\kappa_1 + \frac{1}{\sqrt{\kappa_1^2 - 1}} \arccosh\kappa_1 - \pi \right], \quad \text{with} \quad \kappa_1 = \frac{Z \alpha m_e}{m}. \]

For \( \mu \) this amounts to about 2% correction to the Fermi energy, or, in absolute terms: 0.37465 meV. This is a fairly large effect, and one must consider the next term in Eq. 26, which eventually leads to a Zemach radius correction, \( r_Z(1 + \delta_{2S-\text{hfs}}^{\text{VP1}}) \), see Sec. 5 of the Supplement for more details.

### 2.3.4. Combining VP1 and VP2

We note that this formalism applies to all the vacuum-polarization contributions, including hVP, \( \mu \)VP in \( \mu \), etc. However, in these cases one can expand in \( Z\alpha \) before the \( t \)-integration, which simplifies things a lot. For example, the VP2 and VP1 corrections become equal at leading order, with their combined effect given by:

\[ \delta_{1S-\text{hfs}}^{\text{VP1+VP2}} = \frac{8Z \alpha m_e}{\pi} \int_{t_0}^{\infty} dt \frac{\text{Im}\Pi(t)}{t^{3/2}} + O(Z^2\alpha^3). \]
Plugging in the one-loop VP with a lepton with mass \( m_\ell \), or a charged scalar with mass \( m_\pi \), one obtains: \( \frac{3}{2} Z \alpha^2 (m_\pi/m_\ell) \) and \( \frac{1}{2} Z \alpha^2 (m_\pi/m_\ell) \), respectively. The latter result can be used to estimate the hVP contribution.

3. Evaluations of the forward two-photon exchange

It has been long known (69, 70) that the forward 2\( \gamma \) exchange, Fig. 4(a), is a convenient way to access the order-\( (Z \alpha)^5 \) effects due to inelastic nuclear structure, viz., the polarizability effects. The main ingredient in this calculation is the nuclear Compton scattering amplitude. More specifically, the forward VVCS amplitude which, for a spinless or an unpolarized nucleus with spin, is decomposed into two tensors:

\[
T^\mu\nu (p, q) = \left( -g^\mu\nu + \frac{q^\mu q^\nu}{q^2} \right) T_1 (\nu, Q^2) + \frac{p^\mu p^\nu}{M^2} T_2 (\nu, Q^2),
\]

where \( p \) and \( q \) are the four-momenta of, respectively, the nucleus, with \( p^2 = M^2 \), and the photon. The scalar amplitudes \( T_1 \) and \( T_2 \) are functions of the photon energy and virtuality, \( \nu = p \cdot q/M, \ Q^2 = -q^2 \). A similar decomposition exists for spin-dependent VVCS, which contributes then to the hfs. For a spin-1/2 nucleus there are two spin amplitudes, \( S_1 \) and \( S_2 \). The forward 2\( \gamma \)-exchange contributions to the Lamb shift and hfs have the following generic form:

\[
E^{(2\gamma)}_{nS} = \phi_{nS}^2(0) \sum_{i=1}^2 \int_{0}^{\infty} d\nu \int_{0}^{\infty} dQ^2 K_i(\nu, Q^2) S_i (\nu, Q^2),
\]

\[
E^{(2\gamma)}_{nS-hfs} = \phi_{nS}^2(0) \sum_{i=1}^2 \int_{0}^{\infty} d\nu \int_{0}^{\infty} dQ^2 \tilde{K}_i(\nu, Q^2) S_i (\nu, Q^2),
\]

where \( K_i \) and \( \tilde{K}_i \) are some kernels functions. Further notations and formulae can be found in Refs. 71 and 72, as well as Sec. 4 of the Supplement. In particular, it is important to realize that the Born part of the VVCS amplitudes is expressed in terms of the elastic form factors. It yields the finite-size effects, considered in the previous section, together with the recoil corrections. The non-Born part yields the polarizability contribution. Note that these are not always the same as the elastic and inelastic 2\( \gamma \)-exchange contributions, which refer to the contributions of elastic and inelastic parts of the structure functions.

The VVCS amplitudes can be calculated in \( \chi PT \), but the more traditional approach is the data-driven evaluation using the structure functions. Anticipating the forthcoming discussion, let us remark that the two approaches are presently agreeing on the polarizability contribution to the Lamb shift of \( \mu H \), but disagree for the hfs by several \( \sigma \). The new experimental data on the proton spin structure from the JLab Spin program may be very helpful to resolve the latter discrepancy.

3.1. Lamb shift in \( \mu H \)

The VVCS amplitudes in Eq. 30 are not measurable directly, but can be related to the inclusive scattering data by the fundamental principles of unitarity and causality, viz., the optical theorem and dispersion relations (73, 74, 72). Exploiting the s-channel cut, see Fig. 4(c), one hopes to express everything in terms of the nuclear structure functions. For
the spin-independent amplitudes we have:

\[ T_1(\nu, Q^2) = T_1(0, Q^2) + \frac{32\pi Z^2 \alpha M \nu^2}{Q^2} \int_0^1 \frac{dx}{1 - x^2(\nu/\nu_0)^2 - i0^+} F_1(x, Q^2), \]

\[ T_2(\nu, Q^2) = \frac{16\pi Z^2 \alpha M}{Q^2} \int_0^1 \frac{dx}{1 - x^2(\nu/\nu_0)^2 - i0^+} F_2(x, Q^2), \]

where \( \nu_0 = Q^2/2M \).

Unfortunately, the dispersion relation for \( T_1 \) requires a subtraction, which means not everything is expressed in terms of the structure functions, here \( F_1 \) and \( F_2 \). The amplitude \( T_1(0, Q^2) \), i.e., the subtraction function\(^1\) is an additional unknown in this equation. It is not well-constrained by experimental data, and hence, in a purely data-driven approach its modeling leaves some room for imagination. At the beginning of the proton-radius puzzle, a large subtraction-function contribution was even proposed to resolve the discrepancy (86), yielding the missing 310 µeV in the µH Lamb shift. In all the other existing models, however, this contribution appears to be much smaller, by two orders of magnitude, cf. \( E^{(subt)} \) in Table 1. The modest 2γ-exchange contribution was corroborated by \( \chiPT \) calculations, where this problem of model-dependence does not arise. These results are also displayed in Table 1. Listed in there are the following 2γ-exchange effects in the µH Lamb shift:

- \( E^{(subt)} \) the subtraction function,
- \( E^{(inel)} \) the inelastic structure functions,

\(^1\)The conventional subtraction is done at \( \nu = 0 \), but, a subtraction at \( \nu = iQ \) can be used to diminish the inelastic structure-function contribution and simplify the calculations (85).
\[ E_{(\text{pol})} = E_{(\text{subt})} + E_{(\text{inel})}, \] 
the polarizability contribution,

\[ E_{(\text{el})} \] 
the elastic structure functions (same as the Friar radius with recoil),

\[ E_{(2\gamma)} = E_{(\text{el})} + E_{(\text{pol})}, \] 
the total 2\(\gamma\) exchange.

Despite the moderate effect of the subtraction function, it does constitute the largest uncertainty of the data-driven evaluations. Models of the subtraction function for the proton are constrained at \(Q^2 = 0\) by the magnetic polarizability \(\beta_{M1}\), and at asymptotically large \(Q^2\) by perturbative QCD (78). There is a new idea (87) of how to further constrain it from the dilepton electroproduction \((e^- p \to e^- p e^- e^+)\), but that would be an extremely challenging experiment. There is hope that it can soon be calculated in lattice QCD (88–92, 84).

### 3.2. Hyperfine splitting in H and \(\mu H\)

For the hfs, the 2\(\gamma\)-exchange effects are conventionally split into Zemach-radius, recoil and polarizability contributions (95):

\[
E_{(nS-hfs)} = E_{F_n} \left( \Delta_Z + \Delta_{\text{recoil}} + \Delta_{\text{pol}} \right).
\]

All of these effects begin to contribute at order \((Z\alpha)^5\). While the elastic contributions are known to better than 1\%, the absolute uncertainty of the numerically large Zemach-radius contribution is not negligible. Still, the largest uncertainty comes from the polarizability contribution. In what follows we discuss the Zemach and the polarizability contributions in more detail.

#### 3.2.1. Zemach radius, correlation with the charge radius

The Zemach-radius contribution, defined as \(\Delta_Z = -2Z\alpha m_r r_Z\), can be evaluated based on empirically known form factors using Eq. 14. For example, the recent dispersive analysis of the nucleon electromagnetic form factors from the Bonn group (28) yields:

\[
r_{Zp} = 1.054 \left( ^{+0.003}_{-0.002} \right)_{\text{stat}} \left( ^{+0.000}_{-0.001} \right)_{\text{sys}} \text{ fm}, \quad \Delta_Z(\mu H) = -7403^{+21}_{-16} \text{ ppm}.\]

On the other hand, one can determine this contribution from the experimental hfs, given predictions for the remaining theory contributions. So far we have the measurements of the 1\(S\) hfs in H and the 2\(S\) hfs in \(\mu H\). The corresponding extractions of the Zemach radius are shown in Table 2 and compared with the form-factor determinations. Since baryon \(\chi PT\) (B\(\chi PT\)) gives a smaller prediction for the polarizability contribution than data-driven evaluations, it also gives a smaller Zemach radius. This discrepancy will be discussed below (cf. Figure 6).

There is an appreciable linear correlation between the Zemach and charge radius, illustrated in Fig. 5. The black dashed line represents the usual dipole approximation, \(1/(1+Q^2/\Lambda^2)^2\), for the form factors \(G_E\) and \(G_M\). This correlation is of course more general, given that the proton size is set predominantly by one QCD scale, \(\Lambda_{\text{QCD}}\). Essentially all

| \(ep\) scattering | \(\mu H\) 2\(S\) hfs | H 1\(S\) hfs |
|-------------------|------------------|-----------|
| Lin et al. (28)   | Borah et al. (93)| Antognini et al. (2) |
| 1.054^{+0.003}_{-0.002} | 1.0227(107) | 1.082(37) |
|                   |                  | 1.041(31) |
|                   |                  | 1.045(16) |
|                   |                  | 1.012(14) |

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the empirical parametrizations of the form factors, shown by data points, follow this trend too. For comparison, we show our present determination of $r_{zp}$ from H (blue band) and $r_p$ from $\mu$H (solid red line). The upcoming 1S hfs measurement in $\mu$H is expected to have a big impact on the precise determination of $r_{zp}$.

![Figure 5](image)

Correlation between the Zemach and charge radius of the proton. The shown results are from: Lin et al. (28), Borah et al. (93), CREMA (2), Distler et al. (61), Kelly (96), Bradford et al. (97), Arrington et al. (98), and Arrington & Sick (99).

3.2.2. Polarizability contribution and the spin structure functions. The polarizability contribution is at least an order of magnitude smaller than the Zemach term, but produces a relatively large uncertainty. Here we look at it in more detail. This contribution is usually split into terms, in correspondence with the two spin structure functions, $g_1$ and $g_2$:

$$
\Delta_{\text{pol}} = \Delta_1 + \Delta_2 \equiv \frac{Z\alpha m}{2\pi(1 + \kappa_N)M} \left[ \delta_1 + \delta_2 \right],
$$

34a.

$$
\delta_1 = 18 + \int_0^\infty \frac{dQ}{Q} \kappa_0(Q^2) I_1^{(\text{pol})}(Q^2) + 16M^4 \int_0^\infty \frac{dQ}{Q^3} \int_0^{x_0} dx \kappa_1(x,Q^2) g_1(x,Q^2),
$$

34b.

$$
\delta_2 = 96M^2 \int_0^\infty \frac{dQ}{Q} \int_0^{x_0} dx \kappa_2(x,Q^2) g_2(x,Q^2),
$$

34c.

where $x_0$ is the inelastic threshold, which usually is associated with pion production. The kinematical functions, $\kappa_i$, have a particularly simple form for H, since one may neglect the electron mass,

$$
\kappa_0(Q^2) = 1, \quad \kappa_1(x,Q^2) = \gamma(Q^2/x^2) \left[ 4 + \gamma(Q^2/x^2) \right] - \frac{9}{4}, \quad \kappa_2(x,Q^2) = \gamma(Q^2/x^2) - \frac{1}{2},
$$

35.

with $\gamma(t) \equiv \left( 1 + \sqrt{1 + \frac{4M^2}{t}} \right)^{-1}$. For the more general form see Eq. 37 of the Supplement. Note that only the recoil corrections to the Zemach term are contained in $\Delta_{\text{recoil}}$, whereas the polarizability contribution includes the corresponding recoil effects in itself.

The quantity which stands out in the evaluation of $\Delta_1$ is $I_1^{(\text{pol})}(Q^2)$, which is the polarizability (i.e., non-Born) part of the first moment of $g_1$,

$$
I_1^{(\text{pol})}(Q^2) = I_1(Q^2) + \frac{1}{4} P_2^{(g)}(Q^2), \quad I_1(Q^2) = \frac{2M^2}{Q^2} \int_0^{x_0} dx g_1(x,Q^2),
$$

36.
Table 3  Polarizability contribution to the hfs of H and $\mu$H, in ppm.

| Reference                  | H $\Delta_{\text{pol}}$ | H $\Delta_1$ | H $\Delta_2$ | $\mu$H $\Delta_{\text{pol}}$ | $\mu$H $\Delta_1$ | $\mu$H $\Delta_2$ |
|----------------------------|--------------------------|--------------|--------------|-------------------------------|--------------------|------------------|
| DATA-DRIVEN DISP. EVAL.    |                          |              |              |                               |                    |                  |
| (104) Faustov et al. '06  | 2.2(8)                   | 2.6          | -0.4         | 470(104)                      | 518                | -48              |
| (105, 95) Carlson et al. '11 | 1.88(64)            | 2.00(63)     | -0.13(13)    | 351(114)                      | 370(112)           | -19(19)          |
| (81) Tomalak '18           | 1.91(54)                 | 1.95(95)     | -0.44        | 364(89)                       | 429(84)            | -65(20)          |
| (106) Zielinski '17        | 1.51                     |              |              |                               |                    |                  |
| LEADING-ORDER B$\chi$PT   |                          |              |              |                               |                    |                  |
| (64) Hagelstein et al. '16 | 0.12(55)                 | 0.05(52)     | 0.07(17)     | 37(95)                        | 29(90)             | 9(29)            |
| $+$ $\Delta(1232)$ EXCIT. |                          |              |              |                               |                    |                  |
| (107) Hagelstein et al. '18| -0.16                    | 0.48         | -0.64        | -13                           | 84                 | -97              |

where the Pauli form factor, $F_2(Q^2)$, comes from the non-pole piece of the Born term. There is a large cancellation between the two terms in $I_1^{(\text{pol})}$, which is hard to achieve precisely in empirical evaluations. In fact, at the real-photon point they cancel exactly, $I_1^{(\text{pol})}(0) = 0$, as a consequence of the GDH sum rule (100, 101): $I_1(0) = -\frac{1}{2}k^2_N$. There is also a sum rule for the slope, $I_1^{(\text{pol})}(0)$, relating it to the nucleon spin polarizabilities (102, 103). However, in the data-driven evaluations these relations are only satisfied approximately. In the future, it would be desirable to develop the empirical parametrizations of structure functions with built-in constraints from various sum rules.

The present data-driven evaluations also suffer from the poor knowledge of $g_2$. The data are scarce in the entire kinematic region relevant to $\Delta_2$ (108). The data from the JLab g2p experiment (109–111) may soon improve this situation. Their preliminary data have been used by Zielinski (106) to estimate the effect of $\Delta_2$ in H, see Table 3. In the table, we also show the result of leading-order (LO) B$\chi$PT (64), which finds a relatively small polarizability effect. The uncertainty of the LO calculation is estimated as 30% [$\pm (M_\Delta - M_p)/\text{GeV}$] for the contributions from the longitudinal-transverse and helicity-difference cross sections, $\sigma_{LT}$ and $\sigma_{TT}$, respectively, see Eq. 20 of the Supplement for their relation to the spin structure functions. An inclusion of the $\Delta(1232)$-resonance excitation (107) does not change this situation. It increases the effect in the individual $\Delta_1$ and $\Delta_2$ contributions, but cancels out from the total $\Delta_{\text{pol}}$, as can be seen from comparing the last two rows of the Table. A complete next-to-leading-order B$\chi$PT calculation, as is done for Compton scattering observables (112, 113), is needed here to elucidate this result and

![Figure 6](image_url)

**Figure 6**

The polarizability contribution to the hfs in $\mu$H. For the corresponding values and references, see Table 3.
reduce the uncertainty.

Figure 6 provides a graphic illustration of the present discrepancy between the data-driven evaluations and the LO BχPT. The upcoming 1S hfs measurement in μH will be able to address this discrepancy because, combined with the H, it allows for a separate assessment of the Zemach and polarizability contributions. More details on this separation are given in the following section.

4. Theory updates and future μH experiments

4.1. Lamb shift in μH

The two CREMA measurements of \(2S_{1/2} - 2P_{3/2}^{F=2}\) and \(2S_{1/2} - 2P_{3/2}^{F=0}\) transitions (2) allowed for a determination of the 2S hfs, discussed further-on, and the Lamb shift:

\[
E_{2P-2S}^{exp}(\mu H) = 202.3706 (19)_{stat} (12)_{syst} \text{ meV} = 202.3706 (23)_{total} \text{ meV}. \tag{37}
\]

On the theory side, the updated summary for the μH Lamb shift (taking into account the latest results from Refs. 114, 56, 115, 68) is given in Eq. 38. The most important improvement comes from the NLO calculation of the hVP (68). The accuracy is still limited by the 2γ exchange, finite-size effects and the hVP.

\[
E_{2P-2S}^{exp}(\mu H) = \left[ \frac{205.0074}{\text{Uehling}} + \frac{1.0153}{r_p \text{ indep.}} + \frac{0.0114(3)}{\text{hVP}} + \frac{0.0006(1)}{\text{f.s. corr.}} \right] - \frac{5.2275(10)}{12} \left( \frac{r_p}{\text{fm}} \right)^2 - \frac{E_{2S}^{(2\gamma)}}{2\gamma \text{ exchange}} \right] \text{ meV}, \tag{38}
\]

Using the best data-driven evaluation of the 2γ-exchange (78), \(\Delta E_{2S}^{(2\gamma)} = -33(2) \mu \text{eV}\), we obtain:

\[
r_p(\mu H) = 0.84099(12)_{syst}(23)_{stat}(3)_{hVP}(8)_{f.s.}(23)_{2\gamma \text{fm}} = 0.84099(36) \text{ fm}. \tag{39}
\]

The uncertainty of the radius is limited in equal parts by the precision of the 2S-2P measurements and the prediction of the 2γ-exchange contribution, with the measurement accuracy limited by statistics. The systematic uncertainty of 300 MHz is mainly given by the frequency uncertainty of the laser pulses delivered by the Raman cell, the last stage of the laser system used to generate the pulses at 6 μm. The typical atomic physics systematics such as Stark, collisional and Zeeman shifts are strongly suppressed in the tightly-bound μH atom.

An upgrade of the CREMA-2010 setup (1) holds the potential of improving the 2S-2P measurements by at least a factor of 5, reachable by increasing the statistics by 25 and reducing the systematics by 3. The statistical improvement could be achieved mainly by having a longer data-taking time (from 1 week to 5 weeks), and by increasing the laser pulse energy (from 0.2 mJ to 1 mJ), accompanied by slight overall improvements of the setup, including X-ray detection efficiency, muon beam rate, multi-pass cavity performance and laser repetition rate. The systematic uncertainty could be reduced by using novel optical

The CREMA setup can be upgraded to improve the μH(2S-2P) measurements by a factor 5.
parametric down-conversion technologies under development for the measurement of the hfs in \( \mu \mathrm{H} \). This technology, capable of delivering pulses with few mJ energy and a bandwidth smaller than 100 MHz in the 6 \( \mu \mathrm{m} \) region, enables increasing both the laser pulse energy and the frequency control.

### Principle of the CREMA hfs experiment

The hfs experiment by the CREMA Collaboration follows the sequence illustrated in Fig. 7. A negative muon of 11 MeV/c momentum passes an entrance detector triggering the laser system and is stopped in a \( \mathrm{H}_2 \) gas target (~1 mm thickness, 0.5 bar pressure, 20 K temperature), wherein a \( \mu \mathrm{H} \) atom is formed. While the laser pulse is being generated, the \( \mu \mathrm{H} \) atom is de-exciting to the \( F = 0 \) sublevel (see inset in Fig. 7) of the 1S-state and thermalizing to the \( \mathrm{H}_2 \) gas temperature. After 1 \( \mu \mathrm{s} \), the \( \mu \mathrm{H} \) is thermalized and the generated laser pulse of few-mJ energy at a wavelength of 6.8 \( \mu \mathrm{m} \) (equivalent to a frequency of 44 THz and an energy of 0.18 eV) is coupled into a multi-pass cavity surrounding the muon stopping region. The multiple reflections occurring in this toroidal cavity allow the illumination of a disk-shaped volume with a diameter of 15 mm and a thickness of 0.5 mm with a laser fluence of \( O(10) \) J/cm\(^2\). The on-resonance laser pulse excites the muonic atom from the singlet \( F = 0 \) to the triplet \( F = 1 \) sublevels. Within a short time, an inelastic collisions between the \( \mu \mathrm{H} \) atom and one \( \mathrm{H}_2 \) molecule of the gas target de-excites the \( \mu \mathrm{H} \) atom from the triplet back to the singlet sublevels. In this process, the hfs transition energy is converted into kinetic energy: on average the \( \mu \mathrm{H} \) atom acquires 0.1 eV kinetic energy, the rest goes to the \( \mathrm{H}_2 \) molecule. With this extra kinetic energy, which is much larger than the thermal energy, the \( \mu \mathrm{H} \) atoms start diffusing in the \( \mathrm{H}_2 \) gas reaching the target walls 100 – 400 ns after laser excitation, as shown by the peak in Fig. 7 (right). At the gold-coated target walls the muon is transferred from \( \mu \mathrm{H} \) to the nucleus, forming muonic gold (\( \mu \mathrm{Au}^* \)) in highly excited states. The \( \mu \mathrm{Au}^* \) de-excitation produces various X-rays of MeV energy which are used as signature of a successful laser-induced transition, so that the hfs resonance can be exposed by counting the number of \( \mu \mathrm{Au} \) cascade events after laser excitation as a function of the laser frequency.

### 4.2. Hyperfine splitting in \( \mu \mathrm{H} \)

The improved 2S – 2P measurements discussed above will also improve the precision of the 2S hfs measurement. However, a new level of precision will be reached in the upcoming CREMA measurement of 1S hfs (116). The schematics of this experiment are shown in Fig. 7 explained in the insert. On the theory side, the updated summary for the hfs in \( \mu \mathrm{H} \) is given in Equation 40. Compared with a previous compilation by Peset et al. 7, we have included hVP (117), weak (53), and two-loop eVP corrections in 2\(^{\text{nd}}\) and 3\(^{\text{rd}}\)-order perturbation theory (118), as well as some higher-order radiative corrections (119). For the radius-independent term, we are keeping the error estimate from Refs. 120, which does take into account missing higher-order recoil corrections. The radiative corrections to the 2\( \gamma \) exchange are discussed in Sec. 5 of the Supplement.

Once a high-precision measurement of the 1S hfs in \( \mu \mathrm{H} \) is available, it can be used together with \( \mathrm{H} \) to accurately disentangle the Zeeman and polarizability contributions, \( \Delta_Z \) and \( \Delta_{\text{pol}} \), with unprecedented precision. This is possible because the eVP corrections to the 2\( \gamma \) exchange differ between \( \mathrm{H} \) and \( \mu \mathrm{H} \), cf. Eqs. 40 and 42. Anticipating 1 ppm accuracy for the \( \mu \mathrm{H} \) 1S hfs experiment, the Zeeman radius will be determined with \( 5 \times 10^{-3} \) relative uncertainty and \( \Delta_{\text{pol}}(\mu \mathrm{H}) \) with 40 ppm absolute uncertainty. It will thus lead to the
best empirical determination of the proton Zemach radius from spectroscopy, without the uncertainty associated with the polarizability contribution.

4.3. Pinning down the 1S hyperfine splitting in $\mu$H

The success of the 1S $\mu$H hfs experiments relies critically on the precision and accuracy of the theory prediction. The CREMA Collaboration is expecting 2 hours of data taking time per frequency point to observe an excess of events over background. The 1S hfs resonance would need to be searched in a more than 40 GHz wide frequency range to be compared with a linewidth of about 200 MHz at FWHM resulting from Doppler broadening (60 MHz), laser bandwidth (100 MHz) and collisional effects. We estimate the search range to cover a ±$3\sigma$ band over the present spread of 2γ-exchange theory predictions, cf. Fig. 8. Given the levering radiative corrections allows to disentangle the Zemach radius from H and $\mu$H hfs.
Fractional uncertainty of a quantity $X$: 
$\delta = \sigma_X / X$, with $\sigma_X$ the absolute uncertainty.

limited access to the PSI accelerator facility, it is important to further narrow it down as much as possible.

The $1S$ hfs in H has already been measured with a fractional accuracy of $\delta = 7 \times 10^{-13}$ (121, 122):

$$E_{1S-hfs}^{exp}(H) = 1420.405751768(1) \text{ MHz}.$$ 

The corresponding theory prediction is compiled in Eq. 42. Compared to a previous compilation by Volotka (94), we have recalculated the $\mu$VP correction which agrees with Ref. 123.

We have updated also the hVP, rescaling the recent result obtained for muonium (68). These $\mu$VP and hVP results are considerably larger (roughly by a factor of 3 and 5, respectively) than quoted in (94).

The hyperfine splitting of H (theory update):

$$E_{1S-hfs}^{exp}(H) = \left[ 1418840.082(9) + 1612.673(3) + 0.274 + 0.077 \right] \text{ kHz}$$

$$= -54.430(7) \left[ \frac{r_{\mu\rho}}{\text{fm}} + E_p \left( 0.99807(13) \Delta_{\text{recoil}} + 1.00002 \Delta_{\text{pol}} \right) \right] \text{ kHz}$$

In Refs. 120 and 124, this high-precision hfs measurement was already exploited to constrain the 2γ-exchange contribution and its effect in the hfs of $\mu$H. Here we shall use a somewhat different procedure, where all the uncertainty of rescaling from H to $\mu$H is limited to radiative corrections. Combining the empirical and theoretical values for the $1S$ hfs in H, Eqs. 41 and 42, we deduce a subset of the 2γ-exchange contribution, containing the Zemach radius and polarizability corrections:

$$E_{1S-hfs}^{2\gamma-pol}(H) = E_p(H) \left[ b_{1S}(H) \Delta_Z(H) + c_{1S}(H) \Delta_{\text{pol}}(H) \right] = -54.900(71) \text{ kHz},$$

where $b_{1S}(H) \approx 1 + 2 \times 10^{-5} + 0.01846 - 5\alpha / 4\pi$ and $c_{1S}(H) \approx 1 + 2 \times 10^{-5}$ are the radiative-correction factors shown explicitly in Eq. 42. The correction factors correspond to, respectively, the one-loop eVP correction to the wave function, see Eq. 20, the one-loop eVP insertion in the elastic 2γ-exchange diagram, see Eqs. 43a of the Supplement, as well as self-energy and muon anomalous magnetic moment corrections to the Zemach-radius contribution, see Eq. 45 of the Supplement. We choose not to lump in here the recoil corrections to the Zemach term, because they are known rather precisely. We use (105, 81): $\Delta_{\text{recoil}}(H) = 5.33(5)$ ppm and $\Delta_{\text{recoil}}(\mu H) = 846(6)$ ppm.

To go from H to $\mu$H, we assume that only the radiative factors scale non-trivially with the reduced mass, and that $\Delta_Z$ and $\Delta_{\text{pol}}$ scale linearly:

$$\frac{\Delta_i(H)}{m_r(H)} = \frac{\Delta_i(\mu H)}{m_r(\mu H)}, \quad i = Z, \text{ pol.}$$

This scaling is obvious for the Zemach contribution (cf. Eqs. 15), whereas for the polarizability contribution this has been verified numerically to better than 2% (105). Therefore, the
sum of Zemach radius and polarizability corrections in μH, $E^{Z_{\text{pol}}}_{nS,\text{hfs}}(\mu H)$, can be expressed via the one in the H 1S hfs, $E^{Z_{\text{pol}}}_{1S,\text{hfs}}(H)$, as follows:

$$E^{Z_{\text{pol}}}_{nS,\text{hfs}}(\mu H) = E_F(\mu H) m_e(\mu H) b_{nS}(\mu H) E^{Z_{\text{pol}}}_{1S,\text{hfs}}(H)$$

$$- \frac{E_F(\mu H)}{n^3} \Delta_{\text{pol}}(\mu H) \left[ c_{1S}(H) b_{nS}(\mu H) - c_{nS}(\mu H) \right]$$

where $b_{1S}(H) = 1 + 0.00402 + 0.01846 - 5\alpha/4\pi$, $b_{2S}(H) = 1 + 0.00326 + 0.01846 - 5\alpha/4\pi$, $c_{1S}(\mu H) \approx 1 + 0.00402$, and $c_{2S}(\mu H) \approx 1 + 0.00326$ are the radiative-correction factors shown explicitly in Eq. 40. The second term in Eq. 45 is negligible because the coefficient given by the square brackets is very small. We thus only evaluate the first term and obtain:

$$E^{Z_{\text{pol}}}_{1S,\text{hfs}}(\mu H) = -1.318(2) \text{ meV}, \quad E^{Z_{\text{pol}}}_{2S,\text{hfs}}(\mu H) = -0.1646(2) \text{ meV}. \quad 46.$$  

The main source of uncertainty here is the 2γ recoil contribution $\Delta_{\text{recoil}}(H)$. Adding the 2γ recoil contribution $\Delta_{\text{recoil}}(\mu H)$ to Eq. 46, we obtain a prediction for the full 2γ-exchange contribution to the hfs in μH:

$$E^{(2\gamma)}_{1S,\text{hfs}}(\mu H) = -1.161(2) \text{ meV}, \quad E^{(2\gamma)}_{2S,\text{hfs}}(\mu H) = -0.1450(2) \text{ meV}. \quad 47.$$  

With this, we arrive at a complete prediction of the hfs in μH:

$$E_{1S,\text{hfs}}(\mu H) = 182.636(8) \text{ meV}, \quad E_{2S,\text{hfs}}(\mu H) = 22.8134(9) \text{ meV}, \quad 48.$$  

where we have also included an uncertainty due to possible scaling violation of $\Delta_{\text{pol}}$ at the level of 2% (assuming a very generous size for this contribution, $\Delta_{\text{pol}}(\mu H) = 400 \text{ ppm}$). Our result is shown in Fig. 8, together with the existing μH 2S hfs measurement. The theory predictions based on the empirical hfs in H, Eq. 48, are up to a factor 5 better than results that do not use the H hfs.

Note that all theory predictions shown in Fig. 8 are in agreement, even though the data-driven dispersive evaluations and the BχPT prediction disagree in the polarizability contribution (cf. Fig. 6, Table 3). This is because most works use the experimental H hfs to refine their prediction for the total 2γ-exchange effect. Hence the discrepancy in polarizability is compensated by slightly different Zemach radii.
In future, reversing the above procedure to obtain a prediction of the 2γ-exchange contribution to the 1S hfs in H from a measurement of the 1S hfs in μH, might allow for a benchmark test of the H hfs theory. This, however, would also require further improvements for the recoil corrections from 2γ exchange, as well as for the uncertainty from missing contributions in the μH theory. Note that a slightly better benchmark test \((\delta \sim 2 \times 10^{-9})\) of bound-state QED for a hyperfine transitions can be achieved for the muonium hfs, which the MuSEUM experiment (125) aims to measure with \(\delta \sim 2 \times 10^{-9}\) relative accuracy. To test the muonium hfs on this level, the MuMass experiment (126, 127) has to determine the \(m_\mu/m_e\) ratio to better than \(\delta \sim 1 \times 10^{-9}\) from the 1S-2S transition in muonium.

5. Bound-state QED tests of simple atomic and molecular systems

The simplicity of two- and three-body atomic-molecular systems combined with the precision of laser spectroscopy permit unique confrontations between theory and experiments. The predictive power of bound-state QED, however, depends on the knowledge of fundamental constants such as the masses of the involved particles, \(\alpha\), \(R_\infty\), and nuclear properties such as the nuclear charge radii or magnetic moments.

While the \(\mu\)H and \(\mu\)D measurements have been taken into account in the CODATA-2018 adjustment of the fundamental constants yielding \(r_p = 0.8414(19)\) fm (15), its uncertainty is 5 times larger than the uncertainty from the muonic measurement alone (2), cf. Eq. 39. Hence, the \(r_p\) value from CODATA-2018 does not completely reflect the potential of the \(\mu\)H(2S-2P) measurements. We thus sketch in the following the impact of \(r_p(\mu\)H) by combining it with some selected measurements and corresponding theory predictions in simple systems with distinctive precision and sensitivity. Figure 9 illustrates the impact of the \(\mu\)H spectroscopy and its connection to H, HD\(^+\) and Penning trap measurements that leads to cutting edge tests of bound-state QED for H-like systems, simple molecular systems, and bound-electron g-factors while improving on fundamental constant such as the \(r_p\), \(r_d\), \(R_\infty\), \(m_e\) and \(M_p\). Throughout this section we use the SI units.

5.1. \(\mu\)H to H: testing the H energy levels and extracting \(R_\infty\)

Even though the recent H(2S-8D) measurement (17) is at some tension with the \(\mu\)H results, here we exploit the agreement between the \(r_p\) values from H (19, 18, 21) and \(\mu\)H to illustrate the potential of combining \(\mu\)H and H measurements for testing the H energy levels and improving on \(R_\infty\), the most precisely known fundamental constant and a major player in the adjustment of fundamental constants. \(R_\infty\) also sets the energy scale for atoms, ions and molecules, so that precise predictions of transition frequencies in these systems require its precise value.

In a simplified form, the H energy levels with principal quantum numbers \(n\) and angular momentum \(l\) can be expressed as

\[
f_{nl}^{\text{th}} = -\frac{R_\infty c}{n^2} \left( \frac{1}{1 + \frac{\alpha r_p}{2 \pi}} + \frac{\text{QED}_{nl}}{n^3} + \delta_{10} \frac{\alpha c^4}{3 \pi a_0^4 h^3 n^5} + \ldots \right).
\]

The first term accounts for the Bohr structure corrected for the finite proton mass \(M_p\). The second term \(\text{QED}_{nl}\), scaling dominantly as \(1/n^3\), accounts for radiative, relativistic and higher-order recoil effects while the third term is the finite-size effect. The relevant unknowns in this equation are thus \(R_\infty\) and \(r_p\): in comparison the uncertainties of all the other constants involved can be neglected.
Hence, to determine both \( R_\infty \) and \( r_p \), two transition frequency measurements in \( H \) are needed while QED\(_{nl}\) are taken from theory. When combining the two most precise measurements in \( H \), the \( H(1S-2S) \) transition with precision \( \delta(1S-2S) = 4.2 \times 10^{-15} \) (128) and the \( H(1S-3S) \) transition with precision \( \delta(1S-3S) = 2.5 \times 10^{-11} \) (20), a Rydberg constant with a fractional precision of \( \delta(R_\infty) = 3.5 \times 10^{-12} \) can be obtained.

A more precise \( R_\infty \) value can be determined by combining the \( H(1S-2S) \) with the \( \mu H(2S-2P) \) measurements. Inserting \( r_p(\mu H) \) into the \( H(1S-2S) \) theory prediction:

\[
f^{1\text{th}}_{2S-1S}(\mu H) = \left[ 0.7496091418756 \frac{R_\infty c}{\text{Hz}} - 7126781916(1813) - 1368229 \left( \frac{r_p}{\text{fm}} \right)^2 \right] \text{Hz,}
\]

and comparing it to the measured transition (128):

\[
f^{exp}_{2S-1S}(H) = 2466061413187035(10) \text{ Hz,}
\]

yields a Rydberg constants of

\[
R_\infty c = 3.2898419602509(11) r_p (24)_{\text{H-theory}} \times 10^{15} \text{ Hz,}
\]

with a total uncertainty of 2.7 kHz corresponding to \( \delta(R_\infty) = 8 \times 10^{-13} \). Even though Eq. 50 accounts for several recent updates – hVP (68), two-loop and three-loop QED contributions (129) (e.g., the previously neglected light-by-light contribution \( B_{\text{LbL}}^{1\text{st}}(nS) \) at order \( \alpha^2(Z \alpha)^6 m \ln Z \alpha \), and inelastic three-photon (3\( \gamma \)) exchange (130) – (see Ref. 131 for a recent review) the obtained value is in perfect agreement with Ref. (45, Eq. 22). Notice from Eq. 52 that the \( R_\infty \) accuracy is limited by the uncertainty of the \( H \) theory (2.4 kHz) while the uncertainty from \( r_p(\mu H) \) is only of 1.1 kHz.

A test of the \( H \) energy levels requires combining theory and measurement of three transitions in \( H \): two of them to determine \( R_\infty \) and \( r_p \), the third to check for consistency. This test is presently limited by the uncertainty of the third best measurement in \( H \) (the 1S hfs excluded) and by the correlations of the various contributions to the energy splittings. Hence, a more sensitive way to test the \( H \) energy levels is to use of the precise \( r_p(\mu H) \) value and to combine it with two most precise measurements in \( H \): the \( H(1S-2S) \) and \( H(1S-3S) \) transitions. Agreement between theory and experiment has been verified on the 1 \( \times 10^{-12} \) level, limited by theory.

**5.2. \( \mu^4\text{He}^+ \) and \( \text{He}^+ \): testing higher-order QED and nuclear models**

An interesting test of bound-state QED can be obtained when the ongoing efforts to measure the 1S-2S transition in the hydrogen-like \( \text{He}^+ \) ion in LaserLaB, Amsterdam (37) and MPQ, Garching (38) will be accomplished. To understand the interplay between measurements in \( \text{He}^+ \), \( \mu^4\text{He}^+ \), \( H \) and \( \mu H \) we express the \( \text{He}^+(1S-2S) \) with explicit \( Z \)-dependence:

\[
f^{1\text{th}}_{2S-1S}(\text{He}^+) \approx \frac{3Z^2 c R_\infty}{4} \frac{1}{1 + \frac{m_e}{M_{\alpha}}} + \text{QED}_{\text{He}^+} \left( Z^{3.7}, Z^{5-7} \right) - \frac{7(Z \alpha)c^4}{24\pi a_B^2 h^3} r_{\alpha}^2,
\]

(1 kHz) \hspace{0.5cm} (9 kHz) \hspace{0.5cm} (40 kHz) \hspace{0.5cm} (61 kHz)

with \( M_{\alpha} \) being the alpha-particle mass. The Bohr structure scales only with \( Z^2 \), the finite size with \( Z \), the one-loop QED contributions scale approximately as \( Z^{3.7} \), while the challenging higher-order contributions (e.g., the two-loop \( B_{\text{lo}} \) term at order \( \alpha^2(Z \alpha)^6 m \), the
Figure 9
Simplified scheme showing the impact of $r_p(\mu H)$ on improving fundamental constants and bound-state QED tests.

By considering these uncertainties, it is clear that the 1S-2S transition in He$^+$ can be tested after completion of the measurement in He$^+$ down to an accuracy of $\sim 60$ kHz limited by $r_o$ from $\mu^4$He$^+$. This correspond to a test at the $6 \times 10^{-12}$ level. Even though the energy levels in H are tested on the $1 \times 10^{-12}$ level, He$^+$ has a superior sensitivity to higher-order QED contributions that scale with $Z^5 = 32$ and $Z^6 = 64$.

To push further the QED test in He$^+$ requires reducing the uncertainty of $r_o$, achievable by progressing the 2γ- and 3γ-exchange contributions in $\mu^4$He$^+$. $E^{(2\gamma)A+N}_{2P-2S} = 9.34(20)N(11)\Lambda \text{meV}$ (132), with $A$ and $N$ the nuclear and nucleon contributions, and $E^{(3\gamma)}_{2P-2S} = -0.150(150) \text{meV}$ (10). In order of importance, the 2γ-exchange theory can be advanced by improving on the nucleon-polarizability contribution (primarily the neutron), on the nuclear-polarizability contribution (whose precision is presently limited by the spread from various parametrizations of the nuclear potential), and on the electric form factor needed to compute the elastic part (132, 133).

Conversely, the comparison theory-measurement via Eq. 53a can be used to extract
\( r_\alpha \) to a better precision than from \( \mu^4\text{He}^+ \). With \( r_\alpha \) from \( \text{He}^+ \), the comparison theory-measurement in \( \mu^4\text{He}^+ \) can be used to determine the 2\( \gamma \)-exchange contribution in \( \mu^4\text{He}^+ \) providing a precise benchmark for nuclear theories to guide future advances.

### 5.3. HD\(^+\), \( \text{H}_2^+ \) and \( \text{H}_2 \): from \( r_p \) to \( m_e \) and the bound-electron g-factor

An impressive improvement has been witnessed in recent years in HD\(^+\) theory (134) and experiments (39, 135, 136), so that the precision reached has become sensitive to the proton radius puzzle. The transition frequencies in HD\(^+\) can be expressed as:

\[
f = cR_\infty \left[ K_{NR} \left( \frac{m_e}{M_p} \frac{M_p}{M_d} \right) + \alpha^2 K_{QED} \left( \frac{m_e}{M_p} \frac{M_p}{M_d} \right) + k_p (r_p^2) + k_d (r_d^2) \right].
\]

where the first term corresponds to the non-relativistic energy, the second to QED and relativistic corrections, and the last two terms to finite-size corrections. HD\(^+\) provides thus an independent access to \( R_\infty \), \( m_e/M_p \), \( M_p/M_d \), \( r_p \) and \( r_d \), where \( m_e/M_p \) and \( M_p/M_d \) are electron-to-proton and proton-to-deuteron mass ratios, respectively.

Agreement between theory and experiment in HD\(^+\) has been demonstrated for various transitions (39, 135, 136) down to the \( 10^{-11} \) level, representing the best tests of quantum-three-body predictions. For the rotational transitions presented in Ref. 39 the comparison theory-experiment is limited to the \( 5 \times 10^{-11} \) level by the \( m_e/M_p \) uncertainty while the uncertainties of \( R_\infty \), \( r_p \) and \( r_d \) play a minor role. Nonetheless, the reached precision is sensitive to the proton radius puzzle: the \( r_p \) value from \( \mu \text{H} \) is favoured as it yields to a better agreement between theory and experiment (39).

Conversely, we can equate theory and experiment in HD\(^+\) to extract \( m_e/M_p \) with a fractional precision of \( \delta(m_e/M_p) = 2 \times 10^{-11} \) (39, 135), i.e. a factor of 2 better than achievable combining the electron mass of \( \delta(m_e/M_{12\text{C}^+}) = 3 \times 10^{-11} \) (137) with the proton mass of \( \delta(M_p/M_{12\text{C}^+}) = 3 \times 10^{-11} \) (138) as obtained from Penning traps. The \( m_e/M_p \) ratio from HD\(^+\) can then be combined with \( M_p \) (138) from Penning traps to improve on \( m_e \). This allows an extraction of the electron bound g-factor from the measurement of Ref. 137 to be confronted with corresponding theoretical predictions (139): agreement on the \( 4 \times 10^{-11} \) level is observed, making this the best test of any bound-electron g-factor.

The precision recently reached in HD\(^+\) has established a link between \( r_p \) and the electron, proton, and deuteron masses. The rapid progresses observed in recent years in HD\(^+\) theory and experimental techniques promises a fruitful exploitation of this link that connects two very active precision fields: laser spectroscopy of simple atoms and Penning traps (139). The potential of HD\(^+\) roots in the Hz to kHz line widths given by the tens of milliseconds lifetimes of its ro-vibrational states. This has to be compared with the MHz linewidths of the recently measured 2S-4P and 1S-3S transitions in H. Even higher precision is expected in \( \text{H}_2^+ \) given the day-long lifetimes of its states. Novel quantum-logic schemes and state preparation methods are being developed for this purpose (140). Also spectroscopy of \( \text{H}_2 \), \( \text{D}_2 \) and HD –cornerstones of quantum chemistry– will need soon precise values of \( r_p \) and \( r_d \), expanding the impact of the \( \mu \text{H} \) and \( \mu \text{D} \) measurements to chemical bonds and four-body QED (141, 142).

### 5.4. New Physics searches

Precision spectroscopy of atoms and molecules could sense energy shifts caused by physics beyond the standard model (BSM) involving a low-mass and weakly coupled sector that
escapes detection in high-energy colliders (41, 42, 143). This searches typically involve a comparison between theoretical predictions and experiments that eventually will be limited by hadronic effects. In our context, the explicit way to searches for BSM physics is to look for deviations between $r_p$ values as extracted from the various systems: $ep$ scattering, H, $\mu H$ and molecules. Any deviation might reveal an inconsistency of the theoretical framework pointing to the existence of BSM physics. Presently, these searches are limited by the uncertainty of the $r_p$ as determined from measurements other than $\mu H$.

Along these lines of investigation, Ref. 17 highlights that $R_\infty$ extracted from H tends to decrease as the $n$ of either the upper or lower state increases. Such a trend could be explained by a fifth-force expressed as a Yukawa-like potential with a large length scale (144) mitigating the new tension between $\mu H$ and recent H measurements (17).

A recent study (145) highlighted the peculiar sensitivity of $\mu H$, $\mu D$ and H(1S-2S) to a dark sector with masses in the keV to GeV range. The sensitivity presented in this study is greatly enhanced when accounting for the upcoming measurement of the 1S hfs in $\mu H$, and improved determinations of $r_p$.

The implicit way to exploit $r_p$ for BSM searches, is simply by using its accuracy to improve other fundamental constants increasing the predictive power of our theories. Advancing the 2$\gamma$- and 3$\gamma$-exchange contributions is essential.

### 6. Future prospects

#### Experimental prospects

1. **Precise measurement of the 1S hfs in \( \mu H \):** Three collaborations (CREMA (116), FAMU (50, 51) and J-PARC/Riken (46)) are aiming at a measurement with up to 1 ppm relative precision to extract the 2$\gamma$-exchange contribution. The narrow line width (relative to the 2S-2P splitting) promises improvements in a second phase.

2. **Improved 2S-2P measurements in \( \mu H \):** An upgraded CREMA-2010 setup (1, 2) holds the potential of improving the 2S-2P measurements by at least a factor of 5. This can be obtained principally by increasing the data taking time and using a laser technology capable of delivering mJ-scaled pulses at 6 $\mu$m with bandwidths smaller than 100 MHz under development for the hfs experiment. Improving the 2S-2P measurements by 5, would pave the way for $r_p(\mu H)$ and $R_\infty$ determinations down to $\delta(r_p) \leq 1 \times 10^{-7}$ and $\delta(R_\infty) \leq 1 \times 10^{-13}$, respectively.

3. **He$^+$ 1S-2S measurements (Sec. 5.2):** Two groups (37, 38) are addressing this transition using novel frequency comb and trap technologies. Completion of their experiments will contribute to the proton radius solution and enable testing the higher-order QED contributions (scaling as $Z^{5-7}$) in the He$^+$ ion when assuming $r_\alpha$ from $\mu^4$He$^+$. Conversely, comparing theory to experiment in He$^+$ yields to an alternative and improved determination of $r_\alpha$ that can be used to extract the 2$\gamma$-exchange contribution in $\mu^4$He$^+$ benchmarking nuclear and nucleon models.

4. **Ultra precision-spectroscopy in simple system:** Spectroscopy of H, HD$^+$, H$_2^+$, H$_2$, He, has the potential to not only resolve the proton radius puzzle but to improve fundamental constants and theory tests to unprecedented levels of accuracy.

5. **Proton radius from scattering experiments:** The upgraded PRad experiment (PRad-II) will reduce the experimental uncertainties by a factor of 3.8 and reach down to
the $Q^2$ range of $10^{-5}$ GeV$^2$. The $\mu p$ scattering experiments by the MUSE (PSI) and AMBER (CERN) Collaborations are underway. The PRES Collaboration is building a new experiments in the A2 Hall of MAMI to measure $ep$ scattering using, for the first time, over-determined kinematics, i.e., detecting both the scattered electron and the recoil proton.

6. *Spin structure functions*: Results from the $g2p$ experiment at JLab Hall A (111) will improve evaluations of the polarizability contribution in the $H$ and $\mu H$ hfs.

### Theory prospects

1. **Lattice QCD calculations**: Direct calculations of the nucleon radii using lattice QCD will soon reach the precision comparable to the $ep$ scattering experiments. Also highly anticipated are the lattice calculations of the polarizability effects in the $\mu H$ Lamb shift.

2. **Next-to-leading order $\chi$PT calculations**: The present NLO $\chi$PT calculations, which agree with the wealth of low-energy Compton scattering data, can be extended to muonic atoms, to improve the predictions of the polarizability effect.

3. **Theory prediction of $\mu H$ hfs with ppm accuracy**: The accuracy of the present empirical constraint on the $\mu H$ hfs, see Sec. 4.3, is limited by missing higher-order QED contributions and recoil effects. An improvement in these directions is desirable for finding this transition experimentally and the interpretation of results.

4. **QED for $H$ S-levels**: The two most precise measurements in $H$ are the S-level transitions. They are measured with $\delta(1S-2S) = 4.2 \times 10^{-15}$ (128) and $\delta(1S-3S) = 2.5 \times 10^{-13}$ (20) relative precision, and thus have a smaller uncertainty compared to the uncertainty of the theoretical predictions. An improvement on the theory side will allow for a better extraction of the Rydberg constant and, in turn, better tests of the $H$ energy levels.

5. **Nucleon 2$\gamma$-exchange contribution**: The biggest uncertainty in the $\mu^4He^+$ is presently given by the nucleon 2$\gamma$-exchange contribution. Improving the latter, and in particular the neutron 2$\gamma$-exchange contribution, will allow for an improved extraction of $r_\alpha$, which can then be used for QED tests of $He^+$.

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The authors are not aware of any affiliations, memberships, funding, or financial holdings that might be perceived as affecting the objectivity of this review.

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Supplement to “The proton structure in and out of muonic hydrogen”

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Abstract

In this Supplement, we give a few more details on the theoretical description of nuclear effects in hydrogen-like atoms.
1. Quantum-mechanical Coulomb problem

To set the stage, we recall that the hydrogen energy spectrum:

\[ E_n = -(Z\alpha)^2 m_e/2n^2, \]

with \( m_e = mM/(M + m) \), where \( m, M \) are the masses of the lepton and the nucleus, as well as the corresponding wave functions \( \phi_{nlm}(r) \), are obtained from the Schrödinger equation with the Coulomb potential:

\[
\left[ -\frac{\nabla^2}{2m_e} + V_C(r) - E_n \right] \phi_{nlm}(r) = 0, \quad V_C(r) = -\frac{Z\alpha}{r},
\]

or, in momentum space, from the homogeneous Lippmann-Schwinger equation:

\[
\left( \frac{p^2}{2m_e} - E_n \right) \varphi_{nlm}(p) = \int \frac{dp'}{(2\pi)^3} V_C(p - p') \varphi_{nlm}(p'), \quad V_C(|q|) = -\frac{4\pi Z\alpha}{q^2}.
\]

The coordinate and momentum representations are related via the 3-dimensional Fourier transform. To compute perturbative effects due to a small correction \( V_c(p' - p; \mathbf{p}, \mathbf{p}') \), the following matrix elements are required:

\[
\langle n'l'm' | V_c | nlm \rangle = \int \frac{dp dp'}{(2\pi)^3} V_c(p' - p; \mathbf{p}, \mathbf{p}') \varphi^*_{n'l'm'}(p') \varphi_{nlm}(p).
\]

For a central potential, \( V_c = V_c(|p' - p|) \),

\[
\langle n'l'm' | V_c | nlm \rangle = \delta_{ll'}\delta_{mm'} \int_0^\infty \frac{dq^2}{2\pi^2} V_c(|q|) w_{nl}(q^2),
\]

\[
w_{nl}(q^2) Y_{lm}^*(\Omega_q) \equiv \int dp \varphi^*_{n'l'm'}(p + q) \varphi_{nlm}(p).
\]

For a zero-range correction, \( V_c \) is constant and we are left with

\[
\frac{1}{(2\pi)^3} \int dp \varphi_{nlm}(p) \int dp' \varphi^*_{n'l'm'}(p') = \phi_{nlm}(0) \phi_{n'l'm'}(0) = \frac{(Z\alpha m_e)^3}{\pi(m_e^3)^{3/2}} \delta_{ll'}\delta_{mm'} \delta_{\alpha0}. \]
2. One-photon exchange in dispersive representation

In Sec. 2 of the main Review, we introduced finite-size, polarizability and radiative corrections in hydrogen-like atoms using dispersive representations of the nuclear form factors, the two-photon-exchange potential and the scalar part of the vacuum polarization. In the following subsections, we, firstly, expand on the finite-size effects and express the spherical charge and magnetization distributions through the absorptive parts of the electromagnetic form factors, and secondly, discuss the Uehling contribution.

2.1. Finite-size effects

The spherically-symmetric charge and magnetization distributions, \( \rho_E(r) \) and \( \rho_M(r) \), are Lorentz invariant and related to the form factors and their absorptive parts by, respectively, the Bessel and Laplace transforms. We can see this from the Fourier transforms of the electromagnetic form factors in the Breit frame:

\[
\rho(r) = \int \frac{dq}{(2\pi)^3} G(Q^2) e^{-iq \cdot r} \quad 8a.
\]

\[
= \frac{1}{2\pi^2} \int_0^{\infty} dq Q^2 j_0(Qr) G(Q^2), \quad 8b.
\]

where \( G(Q^2) \) stands for the electric and magnetic Sachs form factors normalized to unity, \( G_E(Q^2) \) and \( G_M(Q^2) \), and \( j_0(Qr) = \frac{\sin Qr}{Qr} \) is the spherical Bessel function. With the dispersive representation of the form factors:

\[
G(Q^2) = \frac{1}{\pi} \int_0^{\infty} dt \frac{\text{Im} G(t)}{t + Q^2 - i0^+}, \quad 9.
\]

and \( t_0 \) the lowest particle-production threshold, it follows in turn that:

\[
\rho_E(r) = \frac{1}{4\pi^2 r} \int_{t_0}^{\infty} dt \text{Im} G_E(t) e^{-r\sqrt{t}}, \quad 10a.
\]

\[
\rho_M(r) = \frac{1}{4\pi^2 r} \int_{t_0}^{\infty} dt \frac{\text{Im} G_M(t)}{1 + \kappa N} e^{-r\sqrt{t}}, \quad 10b.
\]

The finite-size potentials in coordinate space, corresponding to the momentum-space potentials defined in Eqs. 1 and 11 of the main Review, are of Yukawa type:

\[
V_{\text{EFF}}(r) = \frac{Z\alpha}{\pi} \int_{t_0}^{\infty} \frac{dt}{t} \text{Im} G_E(t) \frac{1}{r} e^{-r\sqrt{t}}, \quad 11a.
\]

\[
V_{\text{MFF}}(r) = \frac{Z\alpha}{3\pi m_r M} \left[ F(F+1) - \frac{3}{2} \right] \int_{t_0}^{\infty} dt \text{Im} G_M(t) \frac{1}{r} e^{-r\sqrt{t}}. \quad 11b.
\]

By comparing to Eq. 10b, one can see that \( V_{\text{MFF}}(r) \) is directly proportional to \( \rho_M(r) \). To compute their effect in perturbation theory, as done in Sec. 2 of the main Review, we only need the matrix elements of the Yukawa potential; e.g., at 1\( ^{st} \) order:

\[
\langle nlm | \frac{1}{r} e^{-r\sqrt{t}} | nlm \rangle = \frac{Z\alpha m_r x_n^{l+1}}{n^2 (1 + \sqrt{x_n})^2} \frac{(n + l)!}{(n - l - 1)!(2l + 1)!} 2F_1 \left( 1 + l - n, 2l + 2; x_n; \frac{1}{2} \right), \quad 12.
\]

with \( x_n = (Z\alpha m_r)^2 / (n^2 t) \), and \( 2F_1(a, b; c; x) \) the hypergeometric function of the second kind. For the effect of the \( V_{\text{EFF}}(r) \) potential on the classic \( (2S - 2P) \) Lamb shift, this leads to:

\[
E_{2S-2P}^{(\text{EFF})} \equiv \langle 2S|V_{\text{EFF}}|2S \rangle - \langle 2P|V_{\text{EFF}}|2P \rangle = \frac{(Z\alpha)^4 m_r^3}{2\pi} \int_{t_0}^{\infty} dt \frac{\text{Im} G_E(t)}{(\sqrt{t} + Z\alpha m_r)^4}. \quad 13.
\]
Expanding for $Z\alpha m_r \ll t_0$, one obtains the moments of the charge distribution $\rho_E(r)$, starting with the squared charge radius $\langle r_E^2 \rangle$, cf. Eq. 5 of the main Review. The correction to the HFS from the magnetic form factor, $V_{\text{mFF}}$, is calculated analogously. One obtains the Fermi energy and the magnetic radius as shown in Eq. 12 of the main Review.

### 2.2. Vacuum polarization (Uehling) contribution

The dispersive representation applies to many other effects, such as the vacuum-polarization and self-energy contributions. The former, shown in Fig. 3(a) of the main Review, is obtained simply by replacing $\text{Im} G_E(t)$ with $\text{Im} G(t)$ in the above Eq. 13. For instance, substituting the one-loop eVP,

$$\text{Im} G_E^{(1)}(t) = -\frac{1}{3} \alpha \left(1 + 2m_e^2/t\right) \sqrt{1 - 4m_e^2/t},$$

one obtains (note the convention of the Lamb shift for muonic atoms: 2P-2S),

$$E_{2P-2S}^{\text{eVP}(1)} = \frac{(Z\alpha)^3 m_e^3}{2\pi} \int_{4m_e^2}^{\infty} \frac{dt \ \text{Im} G_E^{(1)}(t)}{(\sqrt{t + Z\alpha m_r})^4} = \frac{\alpha (Z\alpha)^2 m_r}{3k^4} \left(1 + \frac{\kappa (2k^6 - 13k^4 + 44k^2 - 24)}{12\pi(1 - k^2)^2} \right) = \frac{15k^4 - 20k^2 + 8}{4\pi (1 - k^2)^{5/2}} \arccos \kappa,$$

with $\kappa = \frac{Z\alpha m_r}{2m_e}$. For $\mu H$ this gives 205.0074 meV, the well-known Uehling correction. In this example, the integrand cannot be expanded in $Z\alpha$, since $\kappa$ is of order 1, i.e., the Bohr radius is comparable with the Compton wavelength of the virtual $e^+e^-$ pair. For this reason, the Uehling correction is effectively of order $\alpha (Z\alpha)^2$, rather than $\alpha (Z\alpha)^4$ as suggested by naive counting.

### 3. Proton self-energy and the charge-radius definition

Let us briefly consider the correction resulting from the difference between the self-energy of the bound and free proton, see Fig. 3(e) in the main Review. This contribution has the same topology as the finite-size effect, Fig. 3(b) in the main Review, hence, could in principle be absorbed into the proton form factors. The problem is that it differs slightly between H and $\mu H$ and thus requires extra care. This difference is exactly the same for the electric and magnetic form factor (affects only the Dirac form factor), and is proportional to the logarithm of the reduced-mass ratio for the two hydrogens, i.e.,

$$\text{Im} G_{E-\mu H}^H(t) = \text{Im} G_{E-H}^H(t)(t) = Z^2 \alpha \frac{t - 2M^2}{\sqrt{t(t - 4M^2)}} \log \frac{m_e^{(\mu H)}}{m_e^{(H)}}.$$

Using this expression, one can match all of the aforementioned finite-size contributions. For instance, for the charge radius this correction would be:

$$r_p^2(H) - r_p^2(\mu H) = \frac{6}{\pi} \int_{4M^2}^{\infty} dt \frac{\text{Im} G_{E-\mu H}^H(t)}{t^2} = \frac{2Z^2 \alpha}{\pi M^2} \log \frac{m_e^{(\mu H)}}{m_e^{(H)}} = 0.0010737 \text{ fm}^2,$$

which is at the level of the $\mu H$ precision. Presently, this difference is already accounted for (in the charge radius only) by shifting these logarithms, accompanied by the Bethe logarithms.
on the proton line, into the QED contribution, cf. (1, 2). This practice essentially establishes
a unique definition of the charge radius of a bound proton.

The correction shown in Fig. 3(e) is infrared divergent for the free proton and hence the relation to the charge radius extracted from ep scattering depends on the treatment of radiative corrections in these experiments. As these radiative corrections on the proton line are known to be negligibly small (3), at least at the present level of precision of scattering experiments, a possible mismatch with the atomic definition can be ignored.

4. Forward two-photon exchange

![Figure 1](image)

2γ-exchange diagrams in forward kinematics: the horizontal lines correspond to the lepton and the nucleus (bold). (a) Elastic contribution to the 2γ-exchange diagram. (b) Inelastic contribution to the 2γ-exchange diagram, where the “blob” represents all possible excitations. The crossed diagrams are not drawn.

Section 3 of the main Review is dedicated to “Evaluations of the forward two-photon exchange”. In this section, we will introduce the finite-size and polarizability contributions to the Lamb shift and hfs stemming from forward 2γ-exchange, including the lepton mass m, and describe their derivation a bit more detailed. Note that we will limit the discussion to the spin-1/2 case. We will further try to shed light on the often confusing terminology, and present evaluations for the forward 2γ-exchange contributions to the µH hfs, including the Zemach radius and recoil contributions omitted in the review.

4.1. Relation to Compton scattering and electroproduction data

Looking at the forward 2γ-exchange diagrams in Fig. 1, we see that they are related to the process of forward doubly-virtual Compton scattering (VVCS) off a nucleus. Therefore, the forward 2γ-exchange contributions to the Lamb shift and hfs can be written as integrals over the spin-independent and spin-dependent scalar VVCS amplitudes, T_i and S_i, respectively:

\[
E_{nS}^{(2γ)} = 8\pi\alpha m \phi_{nS}^2(0) \int \frac{d^4q}{i(2\pi)^4} \left( \frac{Q^2 - 2\nu^2}{Q^4} \right) T_1(\nu, Q^2) - \left( \frac{Q^2 + \nu^2}{Q^4} \right) T_2(\nu, Q^2),
\]

18a.

\[
E_{nS-hfs}^{(2γ)} = \frac{32\pi\alpha}{3M} \phi_{nS}^2(0) \int \frac{d^4q}{i(2\pi)^4} \left( \frac{Q^2 - \nu^2}{Q^2} \right) S_1(\nu, Q^2) + \frac{3\nu}{M} S_2(\nu, Q^2),
\]

18b.

where M is the nuclear mass, ν is the photon energy in the lab frame, \( q^2 = -Q^2 \) is the photon virtuality, and \( \phi_{nS}^2(0) = 1/(\pi\alpha_B n^3) \) is the wave function at the origin of the atomic nS-level, with \( \alpha_B = 1/(Z\alpha m_e) \) the Bohr radius and \( m_e \) the reduced mass of the atomic bound state. Using a Wick rotation, \( q_0 \rightarrow iQ_0 \), and substituting hyperspherical coordinates, the integrals
simplify to:

\[ E_{\text{NBS}}^{(2\gamma)} = \frac{\alpha}{2\pi^2 m} \phi_{\text{NBS}}^2(0) \int_0^{\infty} \frac{dQ}{Q} \int_0^{\pi} d\chi \sin^2 \chi \times \]

\[ \frac{1 + 2 \cos^2 \chi}{\tau_1 + \cos^2 \chi} T_1(iQ \cos \chi, Q^2) - \sin^2 \chi T_2(iQ \cos \chi, Q^2), \]

\[ E_{\text{NBS-hts}}^{(2\gamma)} = \frac{2\alpha}{3\pi^2 m^2 M} \phi_{\text{NBS}}^2(0) \int_0^{\infty} dQ Q \int_0^{\pi} d\chi \sin^2 \chi \times \]

\[ \frac{2 \cos^2 \chi}{\tau_1 + \cos^2 \chi} S_1(iQ \cos \chi, Q^2) + \frac{3Q \cos \chi}{M} S_2(iQ \cos \chi, Q^2). \]

The VVCS amplitudes can be related to empirical data by applying the general principles of analyticity and causality. In other words, combining the optical theorem:¹

\[ \text{Im} T_1(\nu, Q^2) = \frac{4\pi^2 Z^2 \alpha}{M} F_1(x, Q^2) = \nu \sigma_T(\nu, Q^2), \]

\[ \text{Im} T_2(\nu, Q^2) = \frac{4\pi^2 Z^2 \alpha}{\nu^2 + Q^2} F_2(x, Q^2) = \frac{Q^2 \nu}{\nu^2 + Q^2} \left[ \sigma_T + \sigma_L \right](\nu, Q^2), \]

\[ \text{Im} S_1(\nu, Q^2) = \frac{4\pi^2 Z^2 \alpha M}{\nu^2} g_1(x, Q^2) = \frac{M^2 \nu^2}{\nu^2 + Q^2} \left[ \nu \sigma_{LT} + \sigma_{TT} \right](\nu, Q^2), \]

\[ \text{Im} S_2(\nu, Q^2) = \frac{4\pi^2 Z^2 \alpha M}{\nu^2} g_2(x, Q^2) = \frac{M^2 \nu^2}{\nu^2 + Q^2} \left[ \nu \sigma_{LT} - \sigma_{TT} \right](\nu, Q^2), \]

and dispersion relations, one arrives at:

\[ T_1(\nu, Q^2) - T_1(0, Q^2) = \frac{32\pi^2 Z^2 \alpha M^2}{Q^4} \int_0^1 \frac{dx}{1 - x^2(\nu/\nu_1)^2} F_1(x, Q^2), \]

\[ \left\{ \begin{array}{l} T_2(\nu, Q^2) \\ S_1(\nu, Q^2) \\ S_2(\nu, Q^2) \end{array} \right\} = \frac{16\pi^2 Z \alpha M}{Q^2} \int_0^1 \frac{dx}{1 - x^2(\nu/\nu_1)^2} \left\{ \begin{array}{l} F_2(x, Q^2) \\ g_1(x, Q^2) \\ g_2(x, Q^2) \end{array} \right\}, \]

with \( x = Q^2/2M \nu \), the Bjorken variable, and \( Z \) the nuclear charge (\( Z = 1 \) for the proton). Here, \( F_i(x, Q^2) \) and \( g_i(x, Q^2) \) are the unpolarized and spin structure functions of the nucleus that are directly related to photoabsorption cross sections measurable in lepton-scattering experiments. The cross sections in Eq. 20 are the usual combinations of helicity cross sections: \( \sigma_T = 1/2 (\sigma_{1/2} + \sigma_{3/2}) \) and \( \sigma_{TT} = 1/2 (\sigma_{1/2} - \sigma_{3/2}) \) for transversely polarized photons, and \( \sigma_L = 1/2 (\sigma_{1/2} + \sigma_{1/2}) \) for longitudinally polarized photons, where the subscript on the right-hand-side denotes the total helicity of the \( \gamma^* N \) state. The cross section \( \sigma_{LT} \) describes a simultaneous helicity change of the photon (from longitudinal to transverse) and a nucleon spin-flip.

While the forward \( 2\gamma \)-exchange contribution to the hfs is fully constrained by electro-production data, the contribution to the Lamb shift is not. The high-energy asymptotics of \( F_1(x, Q^2) \), unfortunately, prevent the convergence of an unsubtracted dispersion relation. Therefore, one has to rely on a once-subtracted dispersion relation for \( T_1(\nu, Q^2) \), see Eq. 21a, where the subtraction function \( T_1(0, Q^2) \) is not constrained by data. This introduces an unavoidable model dependence in the data-driven dispersive evaluation of the polarizability contribution to the Lamb shift. In chiral perturbation theory (\( \chi \)PT) calculations this problem does not arise. See Sec. 6 for further details.

¹For discussion of the photon flux factor see Ref. 4. Here we chosen \( K = \nu \).
4.2. Finite-size and polarizability contributions

There are two different criteria that can be used to split the VVCS amplitudes into distinctive contributions. We either consider the simplest tree-level diagrams (aka, the Born diagrams) and everything else (i.e., the non-Born diagrams). Or, we distinguish contributions from the simplest tree-level diagrams which have a pole for the nucleon mass, \( s = M^2 \), (aka, the pole part), and everything else (i.e., the non-pole part). In other words:

\[
T_i(\nu, Q^2) = T_i^{(\text{Born})}(\nu, Q^2) + T_i^{(\text{pole})}(\nu, Q^2) + T_i^{(\text{non-pole})}(\nu, Q^2),
\]

\[
S_i(\nu, Q^2) = S_i^{(\text{Born})}(\nu, Q^2) + S_i^{(\text{pole})}(\nu, Q^2) + S_i^{(\text{non-pole})}(\nu, Q^2),
\]

where the non-Born parts of the VVCS amplitudes are denoted as \( \overline{T}_i \) and \( \overline{S}_i \). The Born and pole contributions are not necessarily the same. For the spin-1/2 case considered here, one finds \( T_2^{(\text{pole})}(\nu, Q^2) = T_2^{(\text{Born})}(\nu, Q^2) \) and \( S_2^{(\text{pole})}(\nu, Q^2) = S_2^{(\text{Born})}(\nu, Q^2) \), but also:

\[
T_1^{(\text{pole})}(\nu, Q^2) = T_1^{(\text{Born})}(\nu, Q^2) + 4\pi Z^2 \frac{\alpha}{M} F_1^2(Q^2),
\]

\[
S_1^{(\text{pole})}(\nu, Q^2) = S_1^{(\text{Born})}(\nu, Q^2) + 2\pi Z^2 \frac{\alpha}{M} F_2^2(Q^2).
\]

Here, \( F_1(Q^2) \) and \( F_2(Q^2) \) are the Dirac and Pauli form factors, related to the electromagnetic Sachs from factors: \( G_E(Q^2) = F_1(Q^2) - \tau F_2(Q^2) \) and \( G_M(Q^2) = F_1(Q^2) + F_2(Q^2) \) with \( \tau = Q^2/4M^2 \). Therefore, one ought to be careful in adding the different contributions to the VVCS amplitudes and 2\( \gamma \) exchange consistently.

Both notations have their advantageous. Speaking in terms of pole and non-pole contributions is convenient if the VVCS amplitudes are expressed as integrals over experimentally observable cross sections by means of dispersion relations, as is done in Eq. 21. In this case, the pole contributions are related to the simple tree-level cross sections of \( \gamma N \rightarrow N \). These 1-particle production cross sections have fixed center-of-mass energy \( s = M^2 \), or equivalently \( x = 1 \). The non-pole contributions are related to inelastic proton structure functions: \( \gamma N \rightarrow \) anything. These are functions of \( x \) and \( Q^2 \), with \( 0 < x < x_0 \) and \( x_0 \) the inelastic threshold, e.g., the threshold for pion-production off the proton: \( x_0 = Q^2/(2M\gamma m_a + m_\pi^2 + Q^2) \).

Speaking in terms of Born and non-Born contributions, on the other hand, allows to conveniently split into finite-size and polarizability contributions. As one can see from Fig. 1, there are contributions to the 2\( \gamma \) exchange, where (a) the nucleus in the intermediate state is intact, and (b) the intermediate state is excited, or a nucleus has been broken up into its constituents. A main focus in the review has been on the polarizability effect, Fig. 1(b), which is defined through the non-Born part of the VVCS amplitudes. Figure 1a) is usually referred to as the elastic 2\( \gamma \)-exchange contribution. It is described through the Born part of the VVCS amplitudes, and attributed to the finite-size effects at order \( (Z\alpha)^3 \).
4.3. Lamb shift formalism

As explained in Sec. 3.1 of the main Review, the 2γ-exchange effect in the Lamb shift is conventionally split into the contribution from elastic structure functions:

\[ E_{nS}^{(el)} = 8(Z\alpha)^2 \phi_{nS}^2(0) \int_0^\infty \frac{dQ}{Q^2} \left[ 4mG_E'(0) - \frac{m}{MQ} \left( \frac{v_1 + 2}{1 + v_1} \right)^2 \left( F_1(Q^2) - 1 \right) \right] \]

with \( G_E'(0) = -(r_2^2)/6 \), and a polarizability contribution \( E_{nS}^{(pol)} \). The latter is the sum of the contributions from inelastic structure functions:

\[ E_{nS}^{(inel)} = -32(Z\alpha)^2 Mm \phi_{nS}^2(0) \int_0^\infty \frac{dQ}{Q^5} \int_0^{x_0} dx \frac{1}{(1 + v_1)(1 + v_x)} \times \]

\[ \left[ \left[ 1 + \frac{v_yv_x}{v_1 + v_x} \right] F_2(x, Q^2) + \frac{2x}{(1 + v_1)(1 + v_x)} \left[ 2 + \frac{v_yv_x}{v_1 + v_x} \right] F_1(x, Q^2) \right], \]

and the non-Born subtraction function:

\[ E_{nS}^{(subt)} = \frac{2am}{\pi} \phi_{nS}^2(0) \int_0^\infty \frac{dQ}{Q^3} \frac{2 + v_1}{(1 + v_1)^2} T_1(0, Q^2). \]

Here, we introduced the following definitions:

\[ v_x = \sqrt{1 + x^2} \tau^{-1}, \quad v = \sqrt{1 + \tau^{-1}}, \quad v_1 = \sqrt{1 + \tau_1^{-1}}, \quad \tau = \frac{Q^2}{4m^2}. \]

Let us sketch how the above formulas are derived. Plugging the dispersion relations from Eq. 21 into Eq. 19a, the nS-level shift generated by the forward 2γ-exchange can be described by:

\[ E_{nS}^{(F_1(x, Q^2))} = -64(Z\alpha)^2 Mm \phi_{nS}^2(0) \int_0^\infty \frac{dQ}{Q^5} \int_0^{x_0} dx \frac{x}{(1 + v_1)^2(1 + v_x)^2} \left[ 2 + \frac{v_yv_x}{v_1 + v_x} \right], \]

\[ E_{nS}^{(F_2(x, Q^2))} = -32(Z\alpha)^2 Mm \phi_{nS}^2(0) \int_0^\infty \frac{dQ}{Q^5} \int_0^{x_0} dx \frac{F_2(x, Q^2)}{(1 + v_1)(1 + v_x)} \left[ 1 + \frac{v_yv_x}{v_1 + v_x} \right], \]

\[ E_{nS}^{(T_1(0, Q^2))} = \frac{2am}{\pi} \phi_{nS}^2(0) \int_0^\infty \frac{dQ}{Q^3} \frac{2 + v_1}{(1 + v_1)^2} T_1(0, Q^2). \]

Now, we need to identify the individual contributions: \( E_{nS}^{(el)} \), \( E_{nS}^{(inel)} \) and \( E_{nS}^{(subt)} \).

To obtain \( E_{nS}^{(inel)} \) in Eq. 25, one has to plug the inelastic structure functions into Eqs. 28a and 28b, where the \( x \) integration goes from 0 to the inelastic threshold \( x_0 \).

To obtain \( E_{nS}^{(subt)} \) in Eq. 26, one has to take into account one subtlety. As one can see from Eq. 26, the so-called subtraction-function contribution conventionally only contains the non-Born part \( T_1(0, Q^2) \) and not the Born part \( T_1^{(Born)}(0, Q^2) \). The latter is treated separately because it is known in terms of elastic form factors:

\[ T_1^{(Born)}(0, Q^2) = \frac{4\pi Z^2\alpha}{M} \left[ G_M(Q^2) - F_1(Q^2) \right]. \]
It is therefore included in $E_{n_S}^{(ei)}$. Note that Eq. 29 also contains the important conversion factor between pole and Born VVCS amplitudes shown in Eq. 23a. To obtain $E_{n_S}^{(ei)}$ in Eq. 24, one then needs Eq. 28c evaluated with Eq. 29, as well as Eqs. 28a and 28b evaluated with the elastic structure functions:

$$F_1^{(el)}(x, Q^2) = \frac{1}{2} G_M^2(Q^2) \delta(1 - x),$$

$$F_2^{(el)}(x, Q^2) = \frac{1}{1 + x} \left[ G_E^2(Q^2) + \tau G_M^2(Q^2) \right] \delta(1 - x).$$

In this way, one will obtain a few contributions that are taken into account already through the one-photon exchange potential. These contributions need to be subtracted in order to avoid double-counting. For one thing, we subtract the contribution of a static, structureless nucleus by replacing $G_i^2(Q^2)$ with $G_i^2(Q^2) - 1$. Furthermore, we subtract the charge-radius term, which is effectively of order-$(Z\alpha)^4$, but disguised as:

$$\frac{16}{3} (Z\alpha)^2 m_r \phi_{n_S}(0) \int_{0}^{\infty} \frac{dQ}{Q^2} \frac{r_E^2}{(r_E^2 + 1)^2}.$$

This leads to $E_{n_S}^{(ei)}$ as given in Eq. 24. See Refs. 5 and 6 for more details.

In Ref. (7), it has been suggested to chose the Euclidean subtraction $T_1(iQ, Q^2)$ instead of the conventional subtraction $T_1(0, Q^2)$ used in Eq. 21a. In this way, one obtains an approximate formula for the proton-polarizability effect in the Lamb shift:

$$E_{n_S}^{(subt)} = \frac{2Z\alpha m}{\pi} \phi_{n_S}(0) \int_{0}^{\infty} \frac{dQ}{Q^2} \frac{2 + v_i}{(1 + v_i)^2} T_1(iQ, Q^2).$$

The remaining contribution of the inelastic structure functions is negligible, due to current conservation (Callan-Gross relation). The single integral in Eq. 32 might hold advantages for future effective field-theory as well as lattice-QCD calculations. See Sec. 6 for further details.

### 4.4. Hyperfine splitting formalism

The dispersive formalism for the hfs is derived analogously. Here, we only give the final formulas. The leading order in $\alpha$ ground-state hfs is given by the Fermi energy:

$$E_F = \frac{8(Z\alpha)^4}{3m^2(1 + \kappa_N)}$$

with $\kappa_N$ the anomalous magnetic moment of the nucleus. The $2\gamma$-exchange effects are proportional to $E_F$, and usually split into three terms:

$$E_{n_S, hfs}^{(2\gamma)} = \frac{E_F}{n^3} (\Delta_Z + \Delta_{recoil} + \Delta_{pol}),$$

referred to as the Zemach-radius, recoil, and polarizability contributions. The former two originate from the so-called elastic $2\gamma$-exchange diagram in Fig. 1 a). They are expressed through the elastic form factors as follows (8):

$$\Delta_Z = \frac{8Z\alpha m_r}{\pi} \int_{0}^{\infty} \frac{dQ}{Q^3} \left[ \frac{G_E(Q^2)G_M(Q^2)}{1 + \kappa_N} - 1 \right] \equiv -2Z\alpha m_v r_Z,$$

$$\Delta_{recoil} = \frac{Z\alpha}{\pi(1 + \kappa_N)} \int_{0}^{\infty} \frac{dQ}{Q} \left[ \frac{G_M(Q^2)}{Q^2} \frac{8mM}{v_i + v} \left( 2F_1(Q^2) + \frac{F_1(Q^2) + 3F_2(Q^2)}{(v_i + 1)(v + 1)} \right) - \frac{8m_r}{v_i + v} \frac{G_M(Q^2)G_E(Q^2)}{Q} \times \frac{M}{1 + v_i} \left( 5 + 4v_i \right) \right].$$
The polarizability contribution originates from the so-called inelastic 2γ-exchange diagram in Fig. 1 b). It can be expressed through the inelastic structure functions \( g_i(x, Q^2) \) and the Pauli form factor \( F_2(Q^2) \):

\[
\Delta_{\text{pol}} = \Delta_1 + \Delta_2 = \frac{Z am}{2\pi(1+\kappa)M} [\delta_1 + \delta_2],
\]

with:

\[
\delta_1 = 2 \int_0^\infty \frac{dQ}{Q} \left( \frac{5 + 4v_t}{(v_t + 1)^2} \left[ 4I_2(Q^2)Z^2 + F_2^2(Q^2) \right] - \frac{32M^4}{Q^4} \int_0^{\xi_0} dx x^2 g_1(x, Q^2) \right)
\]

\[
\delta_2 = 96M^2 \int_0^\infty \frac{dQ}{Q^3} \int_0^{\xi_0} dx g_2(x, Q^2) \frac{1 - v_x}{(1 + v_t)(v_t + v_x)}.
\]

Here, we introduced \( I_1(Q^2) \) as the first moment of the \( g_1 \) structure function:

\[
I_1(Q^2) = \frac{2M^2}{Q^2} \int_0^{\xi_0} dx g_1(x, Q^2),
\]

whose polarizability part reads:

\[
I_1^{(\text{pol})}(Q^2) = I_1(Q^2) + \frac{1}{4} F_2^2(Q^2).
\]

Note that the \( F_2^2(Q^2) \) term is the important conversion factor between pole and Born VVCS amplitudes shown in Eq. 23b. The \( m = 0 \) limit of \( \Delta_{\text{pol}} \) is presented in Sec. 3.2.2 of the main Review, where the polarizability contribution is discussed in details.

In Table 1, we summarize results for the 2γ-exchange contribution to the \( \mu H \) hfs. While \( \Delta_{\text{recoil}} \) is known with the best accuracy, it is a limiting factor when narrowing down the search range for the 1S hfs transition in \( \mu H \) with the help of the precisely measured 1S hfs transition in H, as done in Sec. 4.3 of the main Review.

### 4.5. Off-forward two-photon exchange

As explained in Sec. 2.2 of the main Review, the leading order-(Ze)^5 2γ-exchange corrections originate from the 2γ-exchange diagram in forward kinematics, cf. Fig. 1, while off-forward kinematics (\( t \neq 0 \), i.e., a non-vanishing momentum transfer between initial and final state) are further suppressed in Ze. The forward 2γ-exchange is best described by the dispersive approach introduced above. It can be evaluated based on empirical input for the elastic form factors and inelastic structure functions, and models for the subtraction function, or predicted from \( \chi \)PT.

When considering different contributions of 2γ-exchange type, it is important to distinguish forward and off-forward kinematics and avoid double counting. Take for instance the 2γ-exchange diagrams with \( t \)-channel meson exchanges discussed in Refs. 21–26 for \( \mu H \). Their forward kinematics are already accounted for in the parametrizations of proton structure functions used in the data-driven dispersive approach. Therefore, when combining the recent results for scalar (21, 22), axial-vector (23–25) and tensor (26) mesons exchanges with data-driven evaluations of \( E_n^{(2\gamma)} \), it is important to remove the order-(Ze)^5 effect stemming from the forward limit. To do so, one can apply the once-subtracted coordinate-space
Table 1  Forward $2\gamma$-exchange contribution to the HFS in $\mu H$.

| Reference                        | $\Delta_Z$ [ppm] | $\Delta_{\text{recoil}}$ [ppm] | $\Delta_{\text{pol}}$ [ppm] | $\Delta_1$ [ppm] | $\Delta_2$ [ppm] | $E_{1S,\text{hfs}}^{(2\gamma)}$ [meV] |
|----------------------------------|------------------|--------------------------------|-----------------------------|------------------|------------------|-------------------------------------|
| **DATA-DRIVEN**                  |                  |                                |                             |                  |                  |                                     |
| Pachucki ’96 (1)                 | −8025            | 1666                           | 0(658)                      |                  |                  | −1.160                              |
| Faustov et al. ’01 (9)<sup>a</sup> | −7180            | 410(80)                        | 468                         | −58              |                  |                                     |
| Faustov et al. ’06 (10)<sup>b</sup> | 470(104)         | 518                            | −48                         |                  |                  |                                     |
| Carlson et al. ’11 (11)<sup>c</sup> | −7703            | 931                            | 351(114)                    | −19(19)          | −1.171(39)       |                                     |
| Tomalak ’18 (12)<sup>d</sup>     | −7333(48)        | 846(6)                         | 364(89)                     | 429(84)          | −65(20)          | −1.117(19)                         |
| **HEAVY-BARYON $\chi$PT**        |                  |                                |                             |                  |                  |                                     |
| Peset et al. ’17 (13)            |                  |                                |                             |                  |                  | −1.161(20)                         |
| **LEADING-ORDER $B\chi$PT**      |                  |                                |                             |                  |                  |                                     |
| Hagelstein et al. ’16 (14)       | 37(95)           | 29(90)                         | 9(29)                       |                  |                  |                                     |
| Hagelstein et al. ’18 (15)<sup>e</sup> | −13              | 84                             | −97                         |                  |                  |                                     |

<sup>a</sup>Adjusted values: $\Delta_{\text{pol}}$ and $\Delta_1$ corrected by $−46$ ppm as described in Ref. 16.

<sup>b</sup>Different convention was used to calculate the Pauli form factor contribution to $\Delta_1$, which is equivalent to the approximate formula in the limit of $m = 0$ used for $H$ in Ref. 11.

<sup>c</sup>Elastic form factors from Ref. 17 and updated error analysis from Ref. 16. Note that this result already includes radiative corrections for the Zemach-radius contribution, $(1 + \delta_Z^{\text{rad}})\Delta_Z$ with $\delta_Z^{\text{rad}} \sim 0.0153$ (18, 19), as well as higher-order recoil corrections with the proton anomalous magnetic moment, cf. (11, Eq. 22) and (18).

<sup>d</sup>Uses $r_p$ from $\mu H$ (20) as input.

<sup>e</sup>Partially includes the $\Delta(Z^{1232})$-isobar contribution.

2$\gamma$-exchange potential:

$$V_{2\gamma}(r) = \delta(r) V_{2\gamma}(t = 0) - \frac{1}{\pi} \int_0^\infty \text{d}t \text{ Im} V_{2\gamma}(t) \left[ \frac{\delta(r)}{t} - \frac{e^{-\sqrt{t}r}}{4\pi r} \right].$$

where the $\delta(r)$-function potential, related to the forward limit, is subtracted from the Yukawa potential in the dispersive integral describing the off-forward $2\gamma$ exchange. Note that the pseudoscalar-meson exchanges, on the other hand, are purely off-forward. Thus, their numerically small order-$Z\alpha^6$ effects can be included as they are (14, 27–29).

5. Radiative corrections to spin-dependent two-photon exchange

It is important to include also radiative corrections to the $2\gamma$ exchange. Recently, the initial tension between deuteron charge radius extractions from the $\mu D$ Lamb shift, on the one hand, and the $1S-2S$ H-D isotopic shift paired with the $\mu H$ Lamb shift, on the other hand, was resolved by amending the $\mu D$ theory (30) to include subleading $O(\alpha^6)$ eVP effects (31), as well as inelastic three-photon exchange ($3\gamma$ exchange) (32). Different radiative corrections due to vacuum polarization were discussed in Sec. 2.3 of the main Review. In the following, we will evaluate the eVP insertion in the elastic $2\gamma$-exchange diagram, shown in Fig. 2, for $\mu H$ based on empirical proton form factors.
To a good approximation, the different radiative corrections to the elastic $2\gamma$ exchange considered here can be expressed through numerical scaling factors:

$$E_{nS,\text{hfs}}^{(\text{el})} = \frac{E_F}{n^3} \left( 1 + \frac{\alpha C_1(nS)}{\pi} + \sum_i \delta_{\text{rad},i}^{\text{rad}} \right) \Delta_Z + \left( 1 + \frac{\alpha C_1(nS)}{\pi} + \sum_i \delta_{\text{recoil},i}^{\text{recoil}} \right) \Delta_{\text{recoil}},$$

where $C_1(nS)$ is the eVP correction to the wave function from 2nd-order perturbation theory, see Eq. 20 in the main Review, and $\delta_{\text{rad},i}^{\text{rad}}$ are other radiative corrections. We will denote the correction factors corresponding to the diagram in Fig. 2 at 1st order in perturbation theory by $\delta_{\text{eVP}}^Z$ and $\delta_{\text{eVP}}^\text{recoil}$, respectively.

To account for the insertions of one-loop eVP into the elastic $2\gamma$ exchange, we multiply the integrands in Eqs. 35 and 36 with

$$\Pi_1(Q^2) = \Pi_1(Q^2) - \Pi_1(0) = \frac{\alpha}{\delta \tau_e} \left[ 2 \left( 1 - \frac{1}{2 \tau_e} \right) \left( \sqrt{1 + \frac{1}{\tau_e}} \arccoth \sqrt{1 + \frac{1}{\tau_e}} - 1 \right) + \frac{1}{3} \right],$$

with $\tau_e = Q^2/4m_e^2$ and $m_e$ the electron mass. Several modern proton form factor parametrizations are considered besides the basic dipole form factor: Kelly (33), Bradford et al. (34), Arrington et al. (17), and Borah et al. (35). We find:

$$\delta_{\text{eVP}}^Z = 0.01846(13),$$
$$\delta_{\text{eVP}}^\text{recoil} = 0.01254(4),$$

where the errors cover all form factor parametrizations, including the dipole. The largest corrections are found for the most recent proton form factor parametrization (35), which uses $r_p(\mu_H)$ as a constraint. Our result for $\delta_{\text{eVP}}^Z$ applies to $\mu_H$ and H. It is in good agreement with Ref. 19:

$$\delta_{\text{eVP}}^Z = \frac{\alpha}{3\pi} \left[ 2 \ln \frac{\Lambda^2}{m_e^2} - \frac{634}{315} \right] \sim 0.0182,$$

with the standard value for the dipole form factor of the proton $\Lambda^2 = 0.71$ GeV$^2$. Due to the size of the Zemach-radius contribution, this is an important correction. The $\alpha(Z\alpha)^5$ effect related to $\delta_{\text{recoil}}^{\text{eVP}}$ is relevant as well, since it is slightly larger than the present uncertainty of the pure $(Z\alpha)^5$ $2\gamma$-exchange recoil contribution. It is interesting to note that the eVP recoil correction in H has a different sign, i.e., reduces the recoil contribution: $\delta_{\text{recoil}}^{\text{eVP}}(H) = -0.00195(13)$. For the polarizability contribution from inelastic $2\gamma$ exchange, we expect the eVP correction to be smaller than the present uncertainty. However, it should be included in future calculations, as we aim for an improved prediction of the polarizability contribution.

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For the self-energy and muon anomalous magnetic moment corrections to the Zemach-
radius contribution, we use (19, Eq. 6):

\[ \delta_{Z-\text{line}}^{\mu} = \frac{5\alpha}{4\pi}. \]

The radiative corrections to the muon line found in Ref. (36, 37) for the 2\(\gamma\) finite-nuclear-size contribution are slightly larger in magnitude. As these corrections will become more relevant in the future, an independent cross-check would be desirable. Particular care has to be paid to avoid double counting of contributions that are effectively of lower order.

6. Model-independent predictions of the Lamb shift polarizability contribution

The subtraction function contribution, Eq. 28c, whose \(Q^2\)-dependence is not constrained by data, is the bottleneck of the dispersive approach in the calculation of the Lamb shift polarizability contribution. A systematically improvable calculations is necessary in order to refine the theoretical predictions of the 2\(\gamma\) exchange. In the following, we briefly discuss the prediction from baryon \(\chi\)PT (B\(\chi\)PT), focusing in particular on an updated error estimate for the LO plus \(\Delta(1232)\) isobar prediction (38) (presented in Table 1 of the main Review), as well as future prospects for lattice QCD.

6.1. Chiral perturbation theory

Low-energy effective field-theories, such as B\(\chi\)PT, are expected to be best applicable to atomic systems, where the energies are naturally very small. B\(\chi\)PT is a low-energy effective field-theory of QCD at energies well below 1 GeV. It is formulated in terms of hadronic degrees of freedom; here: pions, nucleons and the lowest nucleon-excitation \(\Delta(1232)\). It has predictive power for the nucleon polarizabilities up to and including NLO. That means all relevant low-energy constants can be matched to other observables. Thus, B\(\chi\)PT is used to make predictions for the non-Born VVCS amplitudes, \(\bar{T}_i\) and \(\bar{S}_i\), and in turn, the proton-polarizability contribution to the Lamb shift and HFS. The main purpose of the predictions from B\(\chi\)PT, discussed below, as well as from heavy-baryon \(\chi\)PT (39, 40), is to provide a consistency check for the dispersive evaluations presented in Sec. 4 and remove model dependence.

In Table 1 of the main Review, we show the LO and LO plus \(\Delta(1232)\) isobar predictions from B\(\chi\)PT (38, 41). A few remarks are in order when it comes to the \(\Delta\)-exchange contributions from B\(\chi\)PT. It is customary to include a dipole form factor on the dominant magnetic coupling of the \(N \to \gamma\Delta\) transition to model a vector-meson type of dependence. It has been shown that in this way B\(\chi\)PT is able to reproduce pion electroproduction data. In addition, we can see from Fig. 4 in Ref. 38 that the B\(\chi\)PT prediction of \(T_1(0, Q^2)/Q^2\) with inclusion of the \(\Delta\) form factor is in better agreement with the empirical super-convergence relation estimate from Ref. 42. Both display a sign change in the region of \(Q^2\) between 0.03 and 0.28 GeV\(^2\). Furthermore, we need to ensure that the contributions to the 2\(\gamma\)-exchange integral from beyond the scale at which B\(\chi\)PT as an effective field-theory is safely applicable do not exceed the expected uncertainty of such calculation. To regularize the behaviour, one can go a step further away from the pure B\(\chi\)PT framework and relate the \(\gamma N\Delta\) couplings to Jones-Scadron form factors (43), which in turn can be related to electromagnetic nucleon form factors through the use of large-\(N_c\) relations (44). This approach has been used in Refs. 15, 38.
In the following, we present an improved error estimate for the LO+Δ prediction described above. The incomplete NLO calculation (missing πΔ loops), as well as the departure from pure BχPT by the use of large-Nc relations and form factors, complicate the error estimate of the theory prediction (38). Our improved error estimate is motivated by the low-energy expansion of the Lamb shift polarizability contribution in terms of the electric and magnetic dipole polarizabilities.

The 2γ-exchange contribution to the Lamb shift is dominated by longitudinal photons and, in turn, the electric dipole polarizability and electric Sachs form factor. Let us start from a low-energy expansion of the spin-independent 2γ contribution:

\[ E^{(2γ)}_{nS} = \frac{α}{π} \varphi_0^2(0) \int_0^∞ \frac{dQ}{Q^2} (\sqrt{τ_1} - \sqrt{1 + τ_1}) T_{L}(0, Q^2) , \]

with the purely longitudinal amplitude:

\[ T_{L}(ν, Q^2) = -T_{1}(ν, Q^2) + (1 + ν^2/Q^2) T_{2}(ν, Q^2) . \]

That the latter is longitudinal follows from Eqs. 20a and 20b. In a next step we consider the low-energy expansion of the non-Born part of the VVCS amplitudes:

\[ \tilde{T}_{1}(0, Q^2) = 4πβ_{M1} Q^2 + O(Q^4) , \quad \tilde{T}_{2}(0, Q^2) = 4π(α_{E1} + β_{M1}) Q^2 + O(Q^4) . \]

and an analogous expansion of the Born part:

\[ T^{(Born)}_{L}(0, Q^2) = \frac{16παm^2}{MQ^2} [G_E^2(Q^2) + O(Q^4)] . \]

Combining Eqs. 48a and 48b into \( \tilde{T}_{L}(0, Q^2) \), we can see that the polarizability contribution to the Lamb shift is indeed dominated by the electric dipole polarizability \( α_{E1} \). Looking at the low-Q part of Eq. 49, confirms that the elastic contribution to the Lamb shift is dominated by the electric Sachs form factor \( G_E(Q^2) \). Equation 48a also shows that the subtraction function is, on the contrary, dominated by transverse photons and the magnetic dipole polarizability \( β_{M1} \). Thus, the dominant polarizability effect must be contained in the inelastic contribution. We can think of the latter as approximated by \( \tilde{T}_{2}(0, Q^2) \), see Ref. (41, Eq. 17), and the sum of dipole polarizabilities.

A leading-order (LO: πN loop) plus next-to-leading-order (NLO: Δ exchange + πΔ loop) BχPT prediction of the static proton polarizabilities reads (in units of \( 10^{-4} \text{ fm}^3 \)) (45):

\[ α^{(p)}_{E1} = 6.8 (\text{πN loop}) - 0.1 (\Delta \text{ exchange}) + 4.5 (\text{πΔ loop}) = 11.2 , \]

\[ β^{(p)}_{M1} = -1.8 (\text{πN loop}) + 7.1 (\Delta \text{ exchange}) - 1.4 (\text{πΔ loop}) = 3.9 . \]

The large contribution of the Δ exchange to \( β_{M1}^{(p)} \) is expected, since the nucleon-to-Delta transition is dominantly of magnetic-dipole type. The subleading Δ exchange, thus, has a negligible effect on the polarizability contribution, but will dominate the subtraction-function contribution. We can see this from Table 1 of the main Review, where Alarcon et al. (41) is the LO BχPT prediction and Lensky et al. (38) is the LO+Δ prediction.

Since polarizability, subtraction-function and inelastic contributions are dominated by \( α_{E1} \), \( β_{M1} \) and their sum, respectively, we can check how well the LO+Δ calculation agrees
with empirical determinations of the static polarizabilities and use this as a criterion for our error estimate. The sum of dipole polarizabilities is constrained by the well known Baldin sum rule (46). It is precisely evaluated for the proton based on empirical total photoabsorption cross sections: \(\alpha_{E1} + \beta_{M1} = 14.0(2) \times 10^{-4} \text{fm}^3\) (47). The PDG recommended values for the individual proton dipole polarizabilities are: \(\alpha_{E1} = 11.2(4) \times 10^{-4} \text{fm}^3\) and \(\beta_{M1} = 2.5(4) \times 10^{-4} \text{fm}^3\) (48). Comparing these empirical values for the static polarizabilities to the LO+\(\Delta\) predictions, we deduce a 53% uncertainty for the subtraction-function contribution towards magnitude decrease, and a 62% uncertainty for the polarizability contribution towards magnitude increase, see Table 1 in the main Review. This is much larger than the usual uncertainty estimate for a LO \(B_{\chi\PT}\) calculation, that would be 15% (~\(m_{\pi}/\text{GeV}\)).

In summary, we can say that the \(B_{\chi\PT}\) and \(HB_{\chi\PT}\) predictions for \(E_{nS}^{(\text{subt})}\) support the model-dependent results used in the dispersive approach. In view of a possible refined measurement of the Lamb shift in \(\mu\text{H}\), the uncertainty of the theoretical 2\(\gamma\)-exchange predictions has to improve further. For a full NLO \(B_{\chi\PT}\) prediction, the contribution of the potentially important \(\pi\Delta\) loops has to be evaluated. In the next subsection, we will discuss the Euclidean subtraction function \(T_1(iQ, Q^2)\) as a new ansatz to calculate the Lamb shift polarizability contribution with prospects for lattice QCD and the NLO \(\pi\Delta\)-loops in \(B_{\chi\PT}\).

### 6.2. Prospects for lattice QCD

An ab-initio calculation of the 2\(\gamma\)-exchange effect would be most desirable. First lattice-QCD results to describe a small part of the 2\(\gamma\)-exchange contribution to the \(\mu\text{H}\) Lamb shift were recently published (49, 50). In the following, we present a different approach that would allow to access most of the 2\(\gamma\)-exchange contribution with a direct lattice-QCD calculation (7). Instead of the conventional subtraction function \(T_1(0, Q^2)\), we suggest to use the Euclidean subtraction function \(T_1(iQ, Q^2)\). It isolates the purely longitudinal amplitude:

\[
T_L(iQ, Q^2) = -T_1(iQ, Q^2) = 4\pi\alpha_{E1}Q^2 + O(Q^4),
\]

thereby, providing an approximate formula for the proton-polarizability effect in the Lamb shift:

\[
E_{nS}^{(\text{subt})} = \frac{2Z\alpha m_e}{\pi} \phi_{nS}(0) \int_0^{x_0} \frac{dQ}{Q^3} \frac{2 + v_i}{(1 + v_i)^2} T_1(iQ, Q^2).
\]

Here, the overline denotes the non-Born or polarizability part of the VVCS amplitudes. The remaining contribution of the inelastic structure functions, as we will show, is negligible. With the subtraction point at \(\nu = iQ\), the \(T_1\) dispersion relation reads as:

\[
T_1(\nu, Q^2) = T_1(iQ, Q^2) + \frac{32\pi\alpha M}{Q^4} (\nu^2 + Q^2) \int_0^1 dx x \frac{F_1(x, Q^2)}{[1 - x^2(\nu/\nu_{el})^2][1 + x^2\tau^{-1}]}.
\]

Obviously, the dispersive integral over the \(F_1(x, Q^2)\) structure function differs from Eq. 21a, thus, also the \(F_1(x, Q^2)\) contribution to the Lamb shift will change. A successive small-\(x\) and low-\(Q\) expansion of the inelastic contribution to the \(nS\)-level shift shows that:

\[
E_{nS}^{(\text{inel})} \sim -16\alpha^2 M\phi_{nS}(0) \int_0^\infty \frac{dQ}{Q^4} \int_0^{x_0} dx F_L(x, Q^2),
\]

where we identified the longitudinal structure function: \(F_L(x, Q^2) = F_2(x, Q^2) - 2xF_1(x, Q^2)\). According to current conservation (or, Callan-Gross relation), the later is...
vanishing for asymptotically low (or large) $Q$, and its moments go as:

$$\lim_{Q^2 \to 0} Q^{-4-2n} \int dx x^{2n} F_L(x, Q^2) = 0.$$  \hspace{1cm} 55.

With the Bosted-Christy parametrization (51) of the structure functions, one can make the rough estimate (7):

$$E_{22}^{(\text{inel})} \approx 1.6 \mu eV.$$  \hspace{1cm} 56.

This shows that the inelastic contribution is indeed negligible at the current level of experimental precision ($\sim 2 \mu eV$), thus, Eq. 52 is a good approximation for the polarizability contribution to the Lamb shift.

The single integral in Eq. 52 holds advantages for effective field-theory as well as lattice-QCD calculations. For one thing, it can be used to calculate the $\pi\Delta$-loop contribution and study the size of contributions from beyond the scale at which B$\chi$PT is safely applicable. For another thing, one could use lattice QCD to calculate $T_1(iQ, Q^2)$. First lattice-QCD calculations of the nucleon VVCS amplitude $T_1(\nu, Q^2)$ in the unphysical region appeared in (52–55).

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