



Two-photon exchange in (muonic) deuterium at N3LO in pionless effective field theory

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Abstract We present a study of the two-photon-exchange (2γ -exchange) corrections to the S -levels in muonic (μD) and ordinary (D) deuterium within the pionless effective field theory ($\not{\pi}$ EFT). Our calculation proceeds up to next-to-next-to-next-to-leading order (N3LO) in the $\not{\pi}$ EFT expansion. The only unknown low-energy constant entering the calculation at this order corresponds to the coupling of a longitudinal photon to the nucleon–nucleon system. To minimise its correlation with the deuteron charge radius, it is extracted using the information about the hydrogen–deuterium isotope shift. We find the elastic 2γ -exchange contribution in μD larger by several standard deviations than obtained in other recent calculations. This discrepancy ameliorates the mismatch between theory and experiment on the size of 2γ -exchange effects, and is attributed to the properties of the deuteron elastic charge form factor parametrisation used to evaluate the elastic contribution. We identify a correlation between the deuteron charge and Friar radii, which can help one to judge how well a form factor parametrisation describes the low-virtuality properties of the deuteron. We also evaluate the higher-order 2γ -exchange contributions in μD , generated by the single-nucleon structure and expected to be the most important terms beyond N3LO. The uncertainty of the theoretical result is dominated by the truncation of the $\not{\pi}$ EFT series and is quantified using a Bayesian approach. The resulting extractions of the deuteron charge radius from the μD Lamb shift, the $2S-1S$ transition in D, and the $2S-1S$ hydrogen–deuterium isotope shift, with the respective 2γ -exchange effects evaluated in a unified $\not{\pi}$ EFT approach, are in perfect agreement.

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1 Introduction

Laser spectroscopy of muonic hydrogen (μH) and deuterium (μD) by the CREMA Collaboration in 2010, 2013 and 2016 enabled determinations of the proton and deuteron charge radii with unprecedented precision:

$$\begin{aligned} r_p(\mu\text{H}) &= 0.84087(26)_{\text{exp}}(29)_{\text{theory}} \text{ fm} \\ &= 0.84087(39) \text{ fm} [1,2], \end{aligned} \quad (1a)$$

$$\begin{aligned} r_d(\mu\text{D}) &= 2.12562(13)_{\text{exp}}(77)_{\text{theory}} \text{ fm} \\ &= 2.12562(78) \text{ fm} [3], \end{aligned} \quad (1b)$$

while the most accurate extraction of the deuteron charge radius,

$$r_d(\mu\text{H} \ \& \ \text{iso}) = 2.12771(22) \text{ fm}, \quad (2)$$

is an indirect achievement combining measurements from the spectroscopy of ordinary and muonic atoms [2]: the $2S$ – $1S$ hydrogen–deuterium (H–D) isotope shift and the Lamb shift in μH . This result is driving the presently recommended value of the deuteron charge radius from the CODATA 2018 report [4]:

$$r_d(\text{CODATA '18}) = 2.12799(74) \text{ fm}. \quad (3)$$

As one can see from Eq. (1), the charge radius extractions are limited by the theory uncertainty, which for muonic atoms is almost solely due to subleading nuclear-structure effects, and in particular, the $O(\alpha^5)$ two-photon exchange (2γ exchange) discussed in this work.

The initial tension between the $r_d(\mu\text{D})$ and $r_d(\mu\text{H} \ \& \ \text{iso})$ extractions, shown above, was resolved in 2019 by amending the μD theory [5] to include the subleading $O(\alpha^6)$ electronic vacuum polarization (VP) effects [6] and the inelastic three-photon exchange (3γ exchange) [7]:

$$\begin{aligned} r_d(\mu\text{D}) &= 2.12710(13)_{\text{exp}}(81)_{\text{theory}} \text{ fm} \\ &= 2.12710(82) \text{ fm} [6]. \end{aligned} \quad (4)$$

The deuteron-radius extractions from deuterium spectroscopy and electron–deuteron (ed) scattering are less precise and lead to larger values:

$$r_d(\text{D spectroscopy}) = 2.1415(45) \text{ fm} [8], \quad (5a)$$

$$r_d(ed \text{ scattering}) = 2.130(10) \text{ fm} [9], \quad (5b)$$

$$r_d(\text{CODATA '14}) = 2.1413(25) \text{ fm} [10]. \quad (5c)$$

This distinct discrepancy for the deuteron radius – the “deuteron radius puzzle” – is strongly affected by the 2γ exchange. It is thus timely to re-evaluate the 2γ -exchange effects in a model-independent manner and try to improve

their precision. While the latest developments [6,7] are certainly important, they do not provide a path to a more systematic improvement of the theory error on the side of nuclear structure.

In this work, we consider the forward 2γ -exchange contributions to D and μD , including the accompanying electronic VP contributions, within the pionless effective field theory ($\not\pi\text{EFT}$) of nuclear forces [11–17]. This framework allows one to represent the nuclear observables in a well-defined perturbation theory, expanding in powers of the small parameter P/m_π , where P is the typical momentum scale (e.g., the size of the relative momentum between two nucleons, or that of the momentum of an external probe) and $m_\pi \simeq 139$ MeV is the pion mass. The typical momentum scale in the deuteron is characterized by the binding momentum $\gamma = \sqrt{M_N B} \simeq 45$ MeV, where M_N is the nucleon mass and B is the deuteron binding energy. The momentum scale probed by the electromagnetic interaction in μD is $\sim \alpha m_\mu$, which is less than an MeV. This is also well below the limiting scale of the theory set by m_π . The atomic systems should thus be well-suited for the application of $\not\pi\text{EFT}$. In addition, it has been shown that $\not\pi\text{EFT}$ provides a good description of low-energy experimental data on real deuteron Compton scattering [18,19], and can be used to investigate the deuteron electric polarizability and electromagnetic form factors (FFs) [15]. Finally, the effective-field-theory (EFT) expansion allows one to quantify the theoretical uncertainty using methods such as Bayesian inference [20]. The basis for our 2γ -exchange calculation is provided in Ref. [21], where closed analytic expressions for the unpolarized amplitudes of forward doubly-virtual Compton scattering (VVCS) off the deuteron are derived.

The paper is organized as follows. In Sect. 2, we briefly introduce the 2γ -exchange and $\not\pi\text{EFT}$ frameworks. In Sect. 3, we calculate the elastic finite-size, inelastic deuteron-polarizability and single-nucleon contributions to the μD Lamb shift, and compare our results to other recent predictions. In Sect. 4, we repeat the same calculation for D and use the H–D isotope shift to fix the unknown low-energy constant (LEC) l_1^{C0s} that enters the VVCS amplitude. In Sect. 5, we utilize the unique possibility to cross-check the theoretical predictions for the 2γ exchange in μD with an empirical determination. The latter is extracted from the measured μD Lamb shift by fixing the deuteron charge radius to the independent value $r_d(\mu\text{H} \ \& \ \text{iso})$. We also compile an update for the theory prediction of the μD Lamb shift that will be used to extract $r_d(\mu\text{D})$ from the measurement of the CREMA Collaboration. In Sect. 6, we discuss deuteron and proton charge radii extractions from μD , D and the H–D isotope shift. A discussion of the neutron charge radius is postponed to Appendix G. In Sect. 7, we finish with conclusion and outlook. The appendices cover: (A) the Bayesian error analysis, (B) the inclusion of nucleon FFs beyond the $\not\pi\text{EFT}$ framework, (C) electronic VP corrections, and updated theory com-

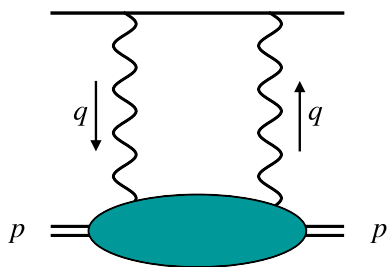


Fig. 1 The leading order in α 2γ -exchange potential

pilations for the: (D) $2S-1S$ H-D isotope shift, (E) $2S-1S$ in H, and (F) $2S-1S$ in D. Appendix E also has a determination of the Rydberg constant R_∞ from $2S-1S$ in H and the Lamb shift in μH . A concise summary of our main results and their implications is published in Ref. [22].

2 Theoretical framework

2.1 2γ exchange in (muonic) deuterium

The leading order (LO) in α 2γ -exchange correction corresponds to the forward kinematics, shown in Fig. 1. It gives a $\delta(\mathbf{r})$ -function correction to the Coulomb potential, thus, only shifts the S -levels, which have a non-vanishing atomic wave function at the origin. The spin-independent forward 2γ exchange is related to the VVCS amplitude off an unpolarized deuteron:

$$T_{fi} = \varepsilon_0 \varepsilon_0'^* f_L(\nu, Q^2) + (\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}'^*) f_T(\nu, Q^2), \tag{6}$$

where $f_L(\nu, Q^2)$ and $f_T(\nu, Q^2)$ are the longitudinal and transverse scalar amplitudes with $Q^2 = -q^2$ and $\nu = \mathbf{p} \cdot \mathbf{q}/M_d$ the photon virtuality and lab frame energy, and M_d the deuteron mass. The modified photon polarization vector components are defined as

$$\begin{aligned} \varepsilon_0 &= \left[\varepsilon_0 - \frac{\nu}{|q|} (\boldsymbol{\varepsilon} \cdot \hat{\mathbf{q}}) \right] \frac{|q|}{Q}, \\ \boldsymbol{\varepsilon} &= \boldsymbol{\varepsilon} - \hat{\mathbf{q}} (\boldsymbol{\varepsilon} \cdot \hat{\mathbf{q}}), \end{aligned} \tag{7}$$

with \mathbf{q} and $\hat{\mathbf{q}} = \mathbf{q}/|q|$ being the photon three-momentum in the lab frame and its unit vector, and $(\varepsilon_0, \boldsymbol{\varepsilon})$ the time and space components of the photon polarization vector. This description in terms of $f_L(\nu, Q^2)$ and $f_T(\nu, Q^2)$ is natural for the \not{A} EFT framework, but not unique. The explicitly covariant tensor decomposition with two other scalar amplitudes $T_i(\nu, Q^2)$ related via

$$\begin{aligned} f_L(\nu, Q^2) &= -T_1(\nu, Q^2) + \left(1 + \frac{\nu^2}{Q^2}\right) T_2(\nu, Q^2), \\ f_T(\nu, Q^2) &= T_1(\nu, Q^2), \end{aligned} \tag{8}$$

is widely used in, e.g., the dispersive 2γ -exchange evaluations [23, 24]. We start from the covariant expression for the forward $O(\alpha^5)$ 2γ -exchange correction to the energy of a nS state in (muonic) deuterium, given in these references, and rewrite them in terms of the longitudinal and transverse amplitudes:

$$\begin{aligned} E_{nS}^{\text{fwd}} &= -8i\pi\alpha m [\phi_n(0)]^2 \int \frac{d^4q}{(2\pi)^4} \\ &\times \frac{(Q^2 - 2\nu^2) T_1(\nu, Q^2) - (Q^2 + \nu^2) T_2(\nu, Q^2)}{Q^4(Q^4 - 4m^2\nu^2)} \end{aligned} \tag{9a}$$

$$\begin{aligned} &= 8i\pi\alpha m [\phi_n(0)]^2 \int \frac{d^4q}{(2\pi)^4} \\ &\times \frac{f_L(\nu, Q^2) + 2(\nu^2/Q^2) f_T(\nu, Q^2)}{Q^2(Q^4 - 4m^2\nu^2)}, \end{aligned} \tag{9b}$$

where m is the electron or muon mass, $[\phi_n(0)]^2 = 1/(\pi n^3 a^3)$ is the (Coulomb) wave function of the nS atomic state at the origin, $a = 1/(\mathcal{Z}\alpha m_r)$ is the Bohr radius, \mathcal{Z} is the nuclear charge ($\mathcal{Z} = 1$ for the deuteron), and $m_r = mM_d/(m + M_d)$ is the atomic reduced mass. Separating the scalar amplitudes into the deuteron-pole and non-pole parts, one splits the 2γ -exchange correction into the elastic and inelastic part [24]. The inelastic part, after doing the Wick rotation $\nu = iq_0$ and introducing the hyperspherical coordinates, takes the form:

$$\begin{aligned} E_{nS}^{\text{inel}} &= -\frac{\alpha}{2\pi^2 m} [\phi_n(0)]^2 \int_0^\infty \frac{dQ}{Q} \int_{-1}^1 dx \sqrt{1-x^2} \\ &\times \frac{f_L(-iQx, Q^2) - 2x^2 f_T(-iQx, Q^2)}{\tau_l + x^2}, \end{aligned} \tag{10}$$

with $\tau_l = Q^2/(4m^2)$. Here we assume that the pole-part is subtracted from the scalar VVCS amplitudes. The elastic part of the 2γ exchange is readily obtained via the deuteron electromagnetic FFs – charge, magnetic, and quadrupole – $G_C(Q^2)$, $G_M(Q^2)$, and $G_Q(Q^2)$, resulting in [24]:

$$\begin{aligned} E_{nS}^{\text{elastic}} &= \frac{m\alpha^2}{M_d(M_d^2 - m^2)} [\phi_n(0)]^2 \int_0^\infty 2 \frac{dQ}{Q} \\ &\times \left\{ \frac{2}{3} G_M^2(Q^2) (1 + \tau_d) \hat{\gamma}_1(\tau_d, \tau_l) \right. \\ &- \left[\frac{G_C^2(Q^2) - 1}{\tau_d} + \frac{2}{3} G_M^2(Q^2) + \frac{8}{9} \tau_d G_Q^2(Q^2) \right] \\ &\times \hat{\gamma}_2(\tau_d, \tau_l) + 16M_d^2 \frac{M_d - m}{Q} G'_C(0) \left. \right\}, \end{aligned} \tag{11}$$

where $\tau_d = Q^2/(4M_d^2)$, and the weighting functions are defined by:

$$\hat{\gamma}_{1,2}(x, y) = \frac{\gamma_{1,2}(x)}{\sqrt{x}} - \frac{\gamma_{1,2}(y)}{\sqrt{y}}, \tag{12a}$$

$$\gamma_1(x) = (1 - 2x)\sqrt{1+x} + 2x^{3/2}, \tag{12b}$$

$$\gamma_2(x) = (1+x)^{3/2} - x^{3/2} - \frac{3}{2}\sqrt{x}. \tag{12c}$$

Note that the contributions of point-like charge and charge radius of the deuteron are removed from the elastic part to avoid double counting [24]. This is done by subtracting the unity and the term proportional to $G'_C(0)$ in Eq. (11).

2.2 Unpolarized deuteron VVCS in pionless EFT

In our analysis, we use results from the $\not{\pi}$ EFT calculation of the unpolarized deuteron VVCS amplitudes $f_L(\nu, Q^2)$ and $f_T(\nu, Q^2)$ presented in Ref. [21]. This section gives a brief recap of the $\not{\pi}$ EFT framework applied to the deuteron VVCS, as well as a description of the technicalities relevant to the 2γ -exchange calculation.

$\not{\pi}$ EFT is an EFT for nucleon interactions at low energies, where the high-energy scale is set by the pion mass m_π . If the momentum transfer between two nucleons is $P \ll m_\pi$, one can treat a pion-exchange interaction as a contact one. In $\not{\pi}$ EFT nucleons are thus interacting through contact interactions [11–13, 15]. The Lagrangian is constructed performing a non-relativistic expansion in the one-nucleon sector and writing out the relevant two-nucleon interactions [11–17]. To assign a particular order to a Feynman graph, one counts powers of momenta [$Q = O(P)$] and energies [$\nu = O(P^2)$] coming from the interaction vertices, nucleon propagators [$O(P^{-2})$], and loops [$O(P^5)$]. The small expansion parameter is the ratio P/m_π . For the deuteron, where the typical momentum scale is the binding momentum γ , this corresponds to $P/m_\pi \simeq 1/3$. Note that different momentum scales can count as different powers of the typical momentum P , depending on the problem setting. For instance, the counting we use has the photon three-momentum $|\mathbf{q}| = O(P)$, whereas its energy is $\nu = O(P^2)$, and hence also its virtuality $Q = O(P)$. This reflects our expectation that the virtual photons in the 2γ -exchange, as viewed in the lab frame, mostly transfer three-momentum, and very little energy, to the intermediate deuteron state, and is in contrast to, e.g., a typical real Compton scattering setting where $\nu = |\mathbf{q}|$, implying they have to be of the same size in the counting.

Regarding the description of the deuteron state, one can use different prescriptions to perform the expansion around the deuteron pole of the nucleon–nucleon (NN) scattering amplitude. The z -parametrisation [17], chosen in Ref. [21, Sec. II B], is particularly well-suited for quantities such as the deuteron electric dipole polarizability α_{E1} that receive

mostly long-range contributions and are thus sensitive to the correct description of the long-range tail of the deuteron wave function. This parametrisation reproduces the residue Z of the NN scattering amplitude at the deuteron pole at next-to-leading order (NLO). The residue is related to the effective range ρ_d in the NN triplet channel via $Z = (1 - \gamma\rho_d)^{-1}$, and is also connected to the asymptotic normalisation of the deuteron S -wave via

$$\psi(r) \xrightarrow{r \rightarrow \infty} \sqrt{\frac{\gamma Z}{2\pi}} \frac{e^{-\gamma r}}{r}. \tag{13}$$

It is therefore straightforward to see that this procedure also reproduces the correct large-distance asymptotics at NLO. Note also that it introduces a new formal expansion parameter $(Z - 1) = O(P)$.

Analysing the counting for the VVCS shows [21, Sec. II B] that the longitudinal amplitude, driven by the deuteron electric polarizability α_{E1} , is dominant, starting at $O(P^{-2})$, whereas the transverse amplitude starts two orders higher at $O(P)$. In the context of the 2γ -exchange correction, Eq. (9b) shows that the f_T contribution is additionally suppressed, compared to the contribution of f_L , by the factor $\nu^2/Q^2 = O(P^2)$. The transverse contribution to the 2γ -exchange correction therefore starts only at $O(P^2)$, or N4LO compared to the leading longitudinal contribution. It is also at N4LO that, as explained in Ref. [21], higher powers of momenta entering the $\not{\pi}$ EFT expansion render the 2γ -exchange correction naively divergent. This divergence ought to be absorbed by a four-nucleon two-lepton contact term entering at this order, and, since there is no data that would allow one to pinpoint the corresponding coupling other than the 2γ -exchange correction itself, this is where the predictive power of $\not{\pi}$ EFT is exhausted. This motivated us to calculate the longitudinal amplitude up to N3LO in Ref. [21]. We also calculated the transverse amplitude up to $O(P)$, or its respective NLO; this allows us to quantify here the corresponding 2γ -exchange contribution.

Further details of the $\not{\pi}$ EFT framework used to calculate f_L and f_T at their respective N3LO and NLO can be found in Ref. [21, Sec. II]. The results for the VVCS amplitudes are given in a closed analytic form in Ref. [21, Sec. III], in terms of the longitudinal and transverse four-point functions $\mathcal{M}_{L,T}(\nu, Q^2)$ and the inverse of the derivative of the deuteron self-energy (SE) at the deuteron pole $[\Sigma'(E_d)]^{-1}$. We use them here to calculate the 2γ -exchange correction. At N3LO in the $\not{\pi}$ EFT expansion of f_L , one encounters a previously undetermined coupling l_1^{C0s} of a longitudinal photon to the two-nucleon system, which contributes, in particular, to $G_C(Q^2)$ and r_d . The latter quantity was used in Ref. [21] to extract l_1^{C0s} from a fit to $r_d(\mu\text{D})$ in Eq. (1b). This procedure is potentially problematic due to the fact that l_1^{C0s} also enters the 2γ -exchange correction, both in μD and the isotope shift.

We investigate the resulting correlations below and demonstrate explicitly that they are negligible at the current level of theoretical and experimental precision.

3 2γ exchange in muonic deuterium

In the following section, we will present in detail our calculation of the elastic and inelastic 2γ-exchange contributions to the Lamb shift in μD. A summary of our results can be found in Sect. 3.4.

3.1 Elastic contribution

We start by considering the elastic contribution to the 2γ-exchange correction based on the $\not\pi$ EFT deuteron FFs. Taking the N3LO result for $G_C(Q^2)$ in Ref. [21, Eq. (75)] and expanding in Eq. (11) also to N3LO results in

$$E_{2S}^{\text{elastic}} = \left[-0.4482 - 0.9938 l_1^{C0s} \right] \text{meV}. \tag{14}$$

This neglects the magnetic and quadrupole FFs, whose contributions are subleading in the $\not\pi$ EFT counting and are indeed numerically very small, see below in Table 2. The electric contact term coupling l_1^{C0s} can be fixed through the deuteron charge radius:

$$r_d^2 \equiv -6 G'_C(0) = \frac{1}{8\gamma^2} + \frac{Z-1}{8\gamma^2} + 2r_0^2 + \frac{3(Z-1)^3}{\gamma^2} l_1^{C0s}, \tag{15}$$

with $r_0^2 = 1/2 \left[r_p^2 + 3/4 M_p^{-2} + r_n^2 \right]$ being the isoscalar nucleon charge radius, with the proton Darwin–Foldy term $3/8 M_p^{-2}$ added to it. Previously, l_1^{C0s} was chosen to reproduce the deuteron charge radius from μD spectroscopy, resulting in [21]

$$l_1^{C0s} = -2.32(41) \times 10^{-3}, \tag{16}$$

where the uncertainty stems from the error of the deuteron radius, Eq. (1b), and the uncertainty of Z . However, the extraction of r_d^2 from μD spectroscopy depends on the theory result for the 2γ-exchange correction (even though the contribution of l_1^{C0s} to the 2γ-exchange correction is small). This correlation can be practically eliminated if the deuteron radius extracted from the combination of the proton radius and the H–D 2S–1S isotope shift, as given in Eq. (2), is used as the reference data point. One has to note that the isotope shift also has a 2γ-exchange contribution, but its relative importance as well as its correlation with r_d^2 is much smaller. To investigate this issue quantitatively, we perform a re-analysis of the isotope shift using the $\not\pi$ EFT formalism to predict the 2γ-exchange correction in ordinary D, see

Sect. 4 and Appendix D. Our calculation confirms that the contribution of l_1^{C0s} to the isotope shift can indeed be safely neglected. The corresponding result for the electric contact term coupling, which will be used throughout this work, is

$$l_1^{C0s} = -1.80(38) \times 10^{-3}. \tag{17}$$

This agrees with the result that we deduced from Eq. (2) [25], but differs from Eq. (16) by about 1 σ, since the extraction via the isotope shift gives a value of $r_d(\mu\text{H \& iso})$ slightly different from $r_d(\mu\text{D})$ in Eq. (1b). The related effect on E_{2S}^{elastic} is small. The final numerical result for the elastic contribution is:

$$\begin{aligned} E_{2S}^{\text{elastic}} &= [-0.2043 - 0.1582 - 0.0626 - 0.0213] \text{meV} \\ &= -0.4463(77) \text{meV}, \end{aligned} \tag{18}$$

where the numbers here stand for the order-by-order contributions. The uncertainty of E_{2S}^{elastic} is due to higher orders in the $\not\pi$ EFT expansion; we quantify it as explained in Appendix A.

To study the elastic (and inelastic) contribution in detail, we split them as shown in Table 1, keeping track of different terms appearing both due to the $(Z-1)$ factors coming from the NLO piece of $[\Sigma'(E_d)]^{-1}$ and due to new sources at each order in the longitudinal four-point function \mathcal{M}_L . This representation will also be useful below in the investigation of the theoretical uncertainty. In order to split the elastic term this way, it is convenient to rewrite the last term in Eq. (11) replacing $G'_C(0)$ by $G_C(0) G'_C(0) = 1/2 [G_C^2(Q^2)]' |_{Q^2=0}$, where the normalization of $G_C(0) = 1$ is used. This reflects the fact that the elastic part of the VVCS amplitude is proportional to the deuteron FFs squared, and allows one to separate the contributions in the integrand without generating spurious singularities at $Q = 0$. One can see from the table that the most important contributions to E_{2S}^{elastic} come, as expected, from the LO part of \mathcal{M}_L , with the nucleon charge radius contributions providing the most important correction at N2LO. One can also see that the only new contributions beyond NLO come either from the nucleon structure or from the N3LO contact term proportional to l_1^{C0s} . The nucleon charge radius contributions may seem somewhat larger than expected at N2LO and N3LO; to judge whether this is an indication of potentially sizeable corrections to E_{2S}^{elastic} beyond N3LO, it is instructive to look at the details of the deuteron charge FF at small photon virtualities. Indeed, it is evident from Eq. (11) that the 2γ-exchange integrand is strongly weighted towards low Q^2 . Therefore, it is the slopes and the curvatures of the deuteron FFs at $Q^2 = 0$ that will have significant influence on the elastic contribution. The slope of the charge FF, proportional to r_d^2 , is reproduced at N3LO; based on that alone, a sizeable modification of the shape of $G_C(Q^2)$ at small Q^2 could come from higher-order coefficients in its expansion

Table 1 E_{2S}^{elastic} , $E_{2S}^{\text{inel},L}$ and their sum E_{2S}^{sum} in detail: contributions appearing at each order in the expansion. Values are in meV. Upper indices indicate the order of \mathcal{M}_L that generates the corresponding contribution, see Ref. [21]. Quantities without labels are the contributions at the respective order excluding the labelled terms listed separately. Labels indicate specific terms within \mathcal{M}_L : r_N^2 , w_2 , P , and I_1^{C0S} stand, in order, for the nucleon charge radii correction, the contribution proportional to the NN triplet S -wave shape parameter w_2 , the NN P -wave contribution, and the contribution proportional to I_1^{C0S}

	E_{2S}^{elastic}	$E_{2S}^{\text{inel},L}$	E_{2S}^{sum}
	LO		
$E^{(-3)}$	-0.2043	-0.9433	-1.1476
	NLO		
$(Z - 1)E^{(-3)}$	-0.1408	-0.6502	-0.7910
$E^{(-2)}$	-0.0174	0.0153	-0.0021
	N2LO		
$(Z - 1)E^{(-2)}$	-0.0120	0.0106	-0.0014
$E^{(-1)}$	0	-0.0006	-0.0006
$E_{r_N^2}^{(-1)}$	-0.0506	0.0389	-0.0117
	N3LO		
$(Z - 1)E^{(-1)}$	0	-0.0004	-0.0004
$(Z - 1)E_{r_N^2}^{(-1)}$	-0.0349	0.0268	-0.0081
$E^{(0)}$	0	-0.0009	-0.0009
$E_{w_2}^{(0)}$		0.0002	0.0002
$E_P^{(0)}$		0.0068	0.0068
$E_{I_1^{C0S}}^{(0)}$	0.0018	-0.0012	0.0006
$E_{r_N^2}^{(0)}$	0.0118	-0.0063	0.0055

in powers of Q^2 . To look into this issue, we review the calculation of E_{2S}^{elastic} using several different deuteron FFs along with the N3LO \not{a} EFT result, and investigate how the features of those FFs affect the result.

Starting with the recent higher-order, N4LO in the respective counting, chiral effective theory (χ ET) calculation of Refs. [26,27], a good agreement between the N3LO \not{a} EFT and the N4LO χ ET results for $G_C(Q^2)$ at low Q was pointed out in Ref. [21]. As expected, our result for E_{2S}^{elastic} perfectly agrees with what one obtains using the χ ET charge FF from Ref. [27]:

$$E_{2S}^{\text{elastic}}(\chi\text{ET}) = -0.4456(18) \text{ meV}, \tag{19}$$

where we neglected the magnetic and quadrupole contributions, and evaluated the uncertainty using the uncertainty of the χ ET result for $G_C(Q^2)$. On the other hand, using the recent empirical deuteron FFs from Ref. [28], Carlson et al. obtained a considerably smaller value [24]:

$$E_{2S}^{\text{elastic}}(\text{emp. FF [28]}) = -0.417(2) \text{ meV}, \tag{20}$$

with the uncertainty estimated using the different FF parametrisations derived in [28]. The same result has been adopted in Ref. [29]. We repeat this calculation, separating the contributions from the charge, magnetic and quadrupole FFs. The results are presented in Table 2 (using parametrisation II of

Abbott et al.), along with values obtained by us based on the Sick and Trautmann parametrisation [9], as well as the χ ET and \not{a} EFT FFs. One can see that the contributions of both the magnetic and quadrupole FFs to the elastic part of the 2γ -exchange correction can be safely neglected at the current level of precision. While the values of E_{2S}^{elastic} obtained in \not{a} EFT, χ ET, and with the Sick and Trautmann parametrisation of the deuteron FF agree, the parametrisation of Abbott et al. gives a significantly smaller value for the elastic contribution. The left panel of Fig. 2 shows that this discrepancy is due to the behaviour of the parametrisation of Ref. [28] being very different from the other three calculations (which would all overlap) at low Q .

Expanding the integrand in Eq. (11) at small Q [neglecting the $G_M(Q^2)$ and $G_Q(Q^2)$ contributions], one obtains

$$\begin{aligned} & \frac{2}{Q} \left[-\frac{G_C^2(Q^2) - 1}{\tau_d} \hat{\gamma}_2(\tau_d, \tau_l) + 16M_d^2 \frac{M_d - m}{Q} G'_C(0) \right] \\ &= 4M_d(M_d - m) \left[4M_d G''_C(0) - 4M_d G'_C(0)^2 \right. \\ & \quad \left. + 3G'_C(0)/m \right] + O(Q). \end{aligned} \tag{21}$$

Therefore, the bulk of the difference can be further traced down to the deuteron charge radius and the 4th moment of the deuteron charge density: $G'_C(0) = -r_d^2/6$ and $G''_C(0) = \langle r_d^4 \rangle / 60$. Also interesting are two further quantities related to

Table 2 Deuteron form factor contributions to the elastic 2γ exchange. Values are in meV. The magnetic and quadrupole contributions are omitted in the χ ET calculation. In $\not\pi$ EFT, those contributions first start at N4LO

Deuteron form factor	G_C	G_M	G_Q	E_{2S}^{elastic}
Abbott et al. [28]	-0.4153	$< 10^{-4}$	-0.0007	-0.417(2) [24]
Sick and Trautmann [9]	-0.4503	$< 10^{-4}$	-0.0006	-0.4509
χ ET N4LO [27]	-0.4456(18)	/	/	-0.4456(18)
$\not\pi$ EFT N3LO	-0.4463(77)	0	0	-0.4463(77)

the elastic 2γ -exchange contribution, namely, the cubic and the Friar radii, defined respectively as [30]:

$$\langle r_d^3 \rangle = \frac{48}{\pi} \int_0^\infty \frac{dQ}{Q^4} \left[G_C(Q^2) - 1 - G'_C(0) Q^2 \right], \quad (22a)$$

$$r_{Fd}^3 = \frac{48}{\pi} \int_0^\infty \frac{dQ}{Q^4} \left[G_C^2(Q^2) - 1 - 2G'_C(0) Q^2 \right]. \quad (22b)$$

In $\not\pi$ EFT at N3LO, the considered moments have the following analytic expressions, obtained using $G_C(Q^2)$ from Ref. [21, Eq. (75)] (note again that the integrand in r_{Fd}^3 has to be expanded up to N3LO):

$$r_{Fd}^3 = \frac{3}{80\gamma^3} \left\{ Z [5 - 2Z(1 - 2 \ln 2)] - \frac{320}{9} r_0^2 \gamma^2 [Z(1 - 4 \ln 2) - 2 + 2 \ln 2] + 80(Z - 1)^3 l_1^{C0s} \right\}, \quad (23a)$$

$$\langle r_d^3 \rangle = \frac{Z}{32\gamma^3} (3 + 32 r_0^2 \gamma^2), \quad (23b)$$

$$\langle r_d^4 \rangle = \frac{Z}{96\gamma^4} (9 + 80 r_0^2 \gamma^2). \quad (23c)$$

Table 3 shows the values of these quantities for the considered FFs. It is evident that parametrisation II of Abbott et al. [28] gives smaller values for all radii. Smaller r_d and $\langle r_d^4 \rangle$ lead to a significantly smaller value of the integrand at low Q , as seen in the left panel of Fig. 2, and consequently a smaller E_{2S}^{elastic} as well as smaller Friar and cubic radii. Note that, neglecting recoil corrections, the elastic contribution can be approximated through the Friar radius as [30]

$$E_{2S}^{\text{elastic, F}} = -\frac{m_r^4 \alpha^5}{24} r_{Fd}^3. \quad (24)$$

This approximation, however, results in a noticeable underestimation of E_{2S}^{elastic} . The $\not\pi$ EFT value, for instance, turns out to be $E_{2S}^{\text{elastic, F}} = -0.4323$ meV, which has to be compared to Eq. (18). We therefore conclude that at the present level of

theoretical precision it is important to retain the full weighting function $\hat{\gamma}_2(\tau_d, \tau_l)$ in Eq. (11) instead of only taking the leading Friar radius term.

The dependence of both r_d^2 and r_{Fd}^3 on l_1^{C0s} can be represented as a linear correlation between these quantities. We show the correlation line in the right panel of Fig. 2, where we also plot a $\pm 1\% \sim (\gamma/m_\pi)^4$ band as a simple estimate of terms beyond N3LO in the $\not\pi$ EFT expansion. One can see that the N4LO χ ET result lies almost on the correlation line, very close to the $\not\pi$ EFT results fixed by the H-D $2S-1S$ isotope shift, see Sect. 4 and Appendix D. The parametrisation of Ref. [9] lies some distance from the line, albeit reasonably close to it, whereas that of Ref. [28] is much further away. It would be interesting to see if this correlation line can be reproduced in a χ ET calculation.

The above considerations indicate that the FF parametrisation of Ref. [28], used in Refs. [24, 29], might not adequately describe the behaviour of the deuteron charge FF at low virtualities. The agreement between the N3LO $\not\pi$ EFT and N4LO χ ET calculations, see Ref. [21, Sec. IV] for a detailed comparison of the FFs, is not entirely surprising as both these EFTs are expected to well reproduce low-momenta/long-range properties of the deuteron, and both calculations are of sufficiently high orders in the respective expansions. This vindicates our choice of the $\not\pi$ EFT as the calculational framework. One can also conclude that the correlation shown in Fig. 2 can serve as a diagnostic criterion for a realistic parametrisation of the deuteron charge FF. Furthermore, one can note that the $\not\pi$ EFT expression for the deuteron charge FF at N3LO, as given in Ref. [21, Sec. IV], can serve as an analytic one-parameter fit to the electron–deuteron scattering data in the low- Q^2 range that is to be covered in the planned DRad experiment [31].

3.2 Inelastic contribution

The calculation of the longitudinal contribution to inelastic part of the 2γ -exchange correction with the known $f_L(\nu, Q^2)$ is straightforward. The only technical complication is that the longitudinal term in the integral of Eq. (10) goes as $f_L(0, Q^2)/Q^3 \propto 1/Q$ for $Q \rightarrow 0$ when one sets $x = 0$. This singularity, however, is spurious, and can be avoided by

Table 3 Various radii corresponding to the different deuteron charge form factors

Radii [fm]	$\not\propto$ EFT N3LO	χ ET N4LO [27]	Sick and Trautmann [9]	Abbott et al. [28]
r_d	2.128	2.126	2.130(10)	2.094(9)
r_{Fd}	3.376	3.372	3.385	3.292
$\langle r_d^3 \rangle^{1/3}$	2.468	2.468	2.480	2.401
$\langle r_d^4 \rangle^{1/4}$	2.820	2.837	2.844	2.726

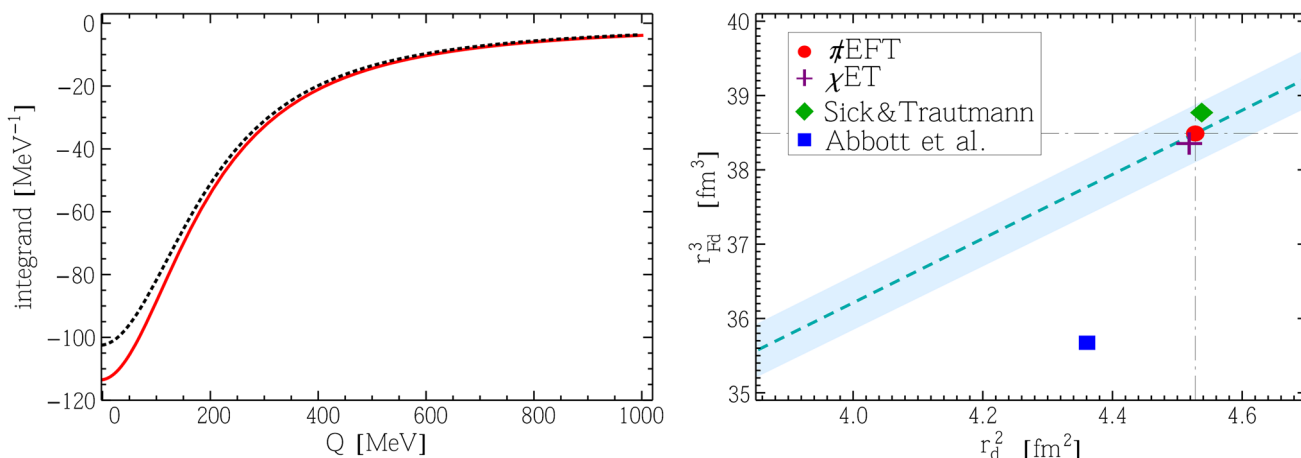


Fig. 2 Left panel: integrand of Eq. (11) as function of Q . Black dotted: deuteron form factor parametrisations from Ref. [28]; red solid: result of the $\not\propto$ EFT calculation. Right panel: correlation of r_{Fd}^3 and r_d^2 . The dashed line shows the correlation obtained from the $\not\propto$ EFT results at N3LO, with the band showing the estimated 1% N3LO uncertainty;

the red disc, purple cross, green diamond, and blue square show the values obtained, respectively, from $\not\propto$ EFT at N3LO, the N4LO χ ET form factor [27], the parametrisation of Ref. [9], and the parametrisation of Ref. [28]

subtracting from $f_L(\nu, Q^2)$ its static part:

$$f_L(\nu, Q^2) = f_L(0, Q^2) + [f_L(\nu, Q^2) - f_L(0, Q^2)]. \quad (25)$$

The integration over x in the integral of $f_L(0, Q^2)$ can be done analytically, resulting in a $f_L(0, Q^2)/Q^2 \propto Q^0$ behaviour for $Q \rightarrow 0$. At the same time, the difference in the square brackets is $O(x^2)$ at small x and therefore cancels the singularity in the weighting function. The longitudinal contribution then results in:

$$E_{2S}^{inel,L} = [-1.5032 + 0.6350 l_1^{C0s}] \text{ meV}. \quad (26)$$

One can see that the coefficients in front of l_1^{C0s} here and in Eq. (14) partially cancel each other. The resulting contribution of the N3LO contact term to the 2γ exchange in μ D is rather small. The numerical order-by-order result for $E_{2S}^{inel,L}$, using l_1^{C0s} as obtained from the H–D isotope shift, is:

$$\begin{aligned} E_{2S}^{inel,L} &= [-0.943 - 0.635 + 0.049 + 0.025] \text{ meV} \\ &= -1.504(16) \text{ meV}. \end{aligned} \quad (27)$$

The uncertainty here is due to higher-order terms in the $\not\propto$ EFT expansion, calculated as explained in Appendix A. The individual terms of the inelastic contribution are shown

in Table 1, in an analogy to what is shown for the elastic part. While the bulk of $E_{2S}^{inel,L}$ is given by the LO part of \mathcal{M}_L , the most important correction comes from the nucleon charge radii, with the second-biggest correction driven by the NLO term of \mathcal{M}_L . The remaining mechanisms all give much smaller contributions.

The above results, Eqs. (26), (27), and Table 1, are obtained with the substitution $|\mathbf{q}| \rightarrow Q$ in the expressions for \mathcal{M}_L ; using $|\mathbf{q}| = \sqrt{Q^2 + \nu^2}$ brings the total value to -1.507 meV. This gives an estimate of the relativistic corrections at N4LO. The smallness of the effect corroborates the choice of counting scheme in our calculation, namely, that the energy transfer is suppressed and $\nu/Q = O(P)$. This statement can be made more quantitative by observing that shrinking the x integration interval in Eq. (10) to $x \in [-\gamma/m_\pi, \gamma/m_\pi] \simeq [-1/3, 1/3]$ retains $\sim 96\%$ of the LO+NLO contribution. Furthermore, the transverse contribution to E_{2S}^{inel} , calculated at NLO for $f_T(\nu, Q^2)$, is small in accordance with the prediction of the $\not\propto$ EFT counting:

$$E_{2S}^{inel,T} = -0.005 \text{ meV}. \quad (28)$$

It is also in a very good agreement with the existing dispersive χ ET-based evaluations [29,32]. Despite the smallness

of the transverse contribution, we add it to the total inelastic contribution, since it is included in most of the alternative calculations, thus having

$$E_{2S}^{\text{inel}} = E_{2S}^{\text{inel},L} + E_{2S}^{\text{inel},T} = -1.509(16) \text{ meV}. \tag{29}$$

The uncertainty of the transverse contribution is neglected.

Based on the observations above, we conclude that the $\not\chi$ EFT counting used by us works well for the present calculation. We also do not expect any higher-order corrections that would change the pattern that one sees at N3LO; a quantification of this statement follows through the Bayesian procedure in Appendix A.

In Table 4, we compare our E_{2S}^{inel} result with other recent evaluations. Our result agrees with the recent covariant dispersive calculation [29] as well as with the value quoted in Ref. [32] within the uncertainties. The latter has a slightly larger in magnitude central value. These two results obtain the deuteron response functions at N3LO in the χ ET expansion to calculate E_{2S}^{inel} from a dispersive integral. The data-driven evaluation of Carlson et al. [24] also uses a dispersive approach, but extracts information on the deuteron response functions from experimental data. It calculates an even larger E_{2S}^{inel} with a large uncertainty that makes it compatible with all other results. In addition, we compare the results in the point-nucleon limit, where the contributions from the nucleon charge radii are removed (in which case we also omit the contribution of l_1^{C0s}). Our result here is compatible with the earlier N3LO χ ET result [32], as well as with that obtained from the N2LO $\not\chi$ EFT deuteron longitudinal response function in the point-nucleon limit [33].

3.3 Single-nucleon effects beyond N3LO

The results of Sects. 3.1 and 3.2 show that single-nucleon contributions generated by the hadron structure, such as the nucleon FFs, are the most important corrections beyond the LO and NLO nuclear-structure effects. They are also potentially the most problematic, since they tend to be enhanced by factors of q^2 compared with the corresponding amplitude with point-like nucleons. For instance, an N4LO correction with two insertions of the nucleon charge radius operator in the LO \mathcal{M}_L diagrams, shown in Ref. [21, Fig. 7], would be enhanced by a factor of q^4 and would lead to a contribution to E_{2S} that is divergent at large Q . Another potentially sizeable single-nucleon effect, first appearing also at N4LO, is that of the nucleon polarizabilities. Their inclusion into the deuteron VVCS amplitude also leads to a similar divergent contribution. A $\not\chi$ EFT consideration would therefore introduce four-nucleon and two-lepton contact terms at N4LO to regularise the divergence generated by the single-nucleon terms. Those contact terms, as pointed out in Sect. 2.2, limit the predictive powers of $\not\chi$ EFT in the study of the 2γ -exchange corrections to N3LO. In this section, we quantify these hadron struc-

ture effects, expected to be the most important ones beyond N3LO, using alternative methods that go beyond the $\not\chi$ EFT expansion.

Starting from the nucleon FF, one alternative that can improve the bad behaviour of the nucleon FF correction would be to insert the full nucleon FFs in the nucleon charge operator vertex, replacing its LO term according to:

$$\frac{1}{2}(1 + \tau_3) \rightarrow \frac{\hat{G}_E^N(Q^2)}{\sqrt{1 + \frac{Q^2}{4M_p^2}}}, \tag{30}$$

where $\hat{G}_E^N(Q^2) = G_E^0(Q^2) + G_E^1(Q^2) \tau_3$ with $G_E^{0,1}$ being the isoscalar and isovector nucleon electric FFs, $G_E^{0,1}(Q^2) = [G_E^p(Q^2) \pm G_E^n(Q^2)]/2$. This procedure obviously represents a departure from the strict $\not\chi$ EFT treatment. It provides, however, a viable workaround and allows one to estimate the effects generated by the higher-order terms in the expansion of the nucleon FFs. It also is routinely used in χ ET calculations of electromagnetic processes in nuclei, since the nucleon FFs do not converge well in a chiral expansion, either, see Refs. [27,29] for recent examples. The specific substitution of Eq. (30), strictly speaking, breaks the electromagnetic gauge invariance. The violating terms are, however, of higher orders than we consider. The modified VVCS amplitudes can be found in Appendix B.

The N3LO $\not\chi$ EFT prediction for the deuteron charge radius, given in Eq. (15), does not change with Eq. (30), as long as we make sure that the parametrisation of the isoscalar nucleon FF agrees with our choice of r_0^2 . We chose the nucleon FF parametrisations from Borah et al. [35], since their slopes are constrained by the nucleon radii used by us: the proton charge radius from μ H spectroscopy given in Eq. (1a), and the neutron charge radius [36,37]:

$$r_n^2 = -0.1161(22) \text{ fm}^2. \tag{31}$$

The elastic 2γ -exchange correction resulting from inserting the full nucleon FFs can be calculated using Eq. (11) with the re-summed deuteron FFs given in Ref. [21, Eqs. (77) and (78)], and it differs only marginally from the result in Eq. (18) (specifically, by about -0.001 meV); we neglect this difference.

The inelastic part changes more significantly. Introducing the nucleon FFs results in the following modifications to the LO and NLO contributions to $E_{2S}^{\text{inel},L}$ in Table 1, using the nucleon FF parametrisation of Ref. [35]:

$$\begin{aligned} E^{(-3)} &\rightarrow E_{\text{FF}}^{(-3)} = -0.9156 \text{ meV}, \\ E^{(-2)} &\rightarrow E_{\text{FF}}^{(-2)} = 0.0125 \text{ meV}, \end{aligned} \tag{32}$$

Table 4 Comparison of our results with other recent calculations for the inelastic contribution E_{2S}^{inel} and the inelastic contribution in the point-nucleon limit $E_{2S}^{\text{inel, p.N.}}$. The latter is the inelastic contribution with point-like nucleons (calculated up to N3LO, with the contribution of l_1^{C0S} omitted). Values are in meV. To compare with Ref. [32], we sub-

	$\not{\chi}$ EFT N3LO	Acharya et al. [29]	Hernandez et al. [32]	Emmons et al. [33]	Carlson et al. [24]
E_{2S}^{inel}	-1.509(16)	-1.511(12)	-1.531(12)		-1.566(740)
$E_{2S}^{\text{inel, p.N.}}$	-1.567		-1.571	-1.574(80)	

Table 5 Single-nucleon subtraction-function contributions from 2γ exchange between muon and proton (μH) or neutron (μn), respectively. The last column gives the $E_{2S}^{\text{hadr, subt}}$ contribution to μD , obtained by rescaling the muon-nucleon values. Values are in meV

	μH	μn	μD
χ PT [39,40]	0.0035(26)	0.0043(25)	0.0091(60)
data-driven	0.0023(13) [41]	0.0043(20) [41]	0.0078(37)

which at the same time absorbs both $E_{r_N^2}^{(-1)}$ and $E_{r_N^2}^{(0)}$. Using a different nucleon FF parametrisation [38] results in:

$$\begin{aligned} E^{(-3)} &\rightarrow E_{\text{FF}}^{(-3)} = -0.9151 \text{ meV}, \\ E^{(-2)} &\rightarrow E_{\text{FF}}^{(-2)} = 0.0125 \text{ meV}. \end{aligned} \tag{33}$$

This amounts to a correction of $E_{2S}^{\text{hadr, FF}} = -0.0129 \text{ meV}$ with the nucleon FFs from Ref. [35]; the parametrisation of Ref. [38] gives $E_{2S}^{\text{hadr, FF}} = -0.0121 \text{ meV}$. In the following, we will adopt

$$E_{2S}^{\text{hadr, FF}} = -0.013(1) \text{ meV}. \tag{34}$$

This effect is within our N3LO uncertainty estimate; one can also notice that it is significantly larger than a similar difference obtained in a χ ET calculation replacing linearised (expanded in Q^2) nucleon FFs by a realistic parametrisation [29]. At the same time, the difference due to the different nucleon FF parametrisations is negligibly small. The replacement of the charge operator by the nucleon FFs in the contributions to $E_{2S}^{\text{inel, L}}$ beyond NLO would also give a negligible effect on the total result.

Coming to the other effect we consider here, that of the nucleon polarizabilities, it consists of two parts, the inelastic and the subtraction hadronic corrections. The first one of the two can be calculated from a dispersive relation, using the empirical deuteron structure functions, at energies starting from the pion production threshold, as done in Ref. [24]:

$$E_{2S}^{\text{hadr, inel}} = -0.028(2) \text{ meV}. \tag{35}$$

tract the subleading $O(\alpha^6 \log \alpha)$ Coulomb correction from their “ η -less” result. The uncertainty given here for their prediction is obtained using the relative uncertainties of individual error sources from Ref. [34, Table 8] (nuclear model, isospin symmetry breaking, relativistic, higher $Z\alpha$) summed in quadrature. The value quoted for Ref. [33] is their “ Z_d -improved” result

See also Ref. [42] for a similar evaluation. Another method to calculate it, similar to inserting the nucleon FFs in the consideration above, is to apply a rescaling procedure to the inelastic 2γ -exchange effect in μH and the analogous inelastic 2γ -exchange effect between a muon and a neutron (μn), adding them together and correcting for the different atomic wave functions, rescaling the sum by the factor $[\phi_{2S}^{\mu\text{D}}(0)/\phi_{2S}^{\mu\text{H}}(0)]^2$, as done in Ref. [5] and references therein. Using the single-nucleon values from Ref. [41], we obtain a value of $-0.030(2) \text{ meV}$, where we added uncertainties linearly to be conservative. This perfectly agrees with the dispersive evaluation given by Eq. (35), which is an indication that the rescaling procedure works well in this setting.

The second part of the single-nucleon polarizability effect, the subtraction contribution, cannot be directly related to empirical data. It has to be either modelled or predicted from baryon chiral perturbation theory (χ PT). With the rescaling procedure described above, and the covariant χ PT results for the proton VVCS subtraction function [40] and its neutron counterpart, we obtain for the subtraction-function contribution to μD ¹:

$$E_{2S}^{\text{hadr, subt}} = 0.009(6) \text{ meV}, \tag{36}$$

which agrees well with the value adopted in Ref. [5]: $0.0098(98) \text{ meV}$. As one can see from Table 5, our predictions agree with the dispersive estimates from Ref. [41]. It is also instructive to compare our result for the proton subtraction contribution, $0.0035(26) \text{ meV}$, to predictions in the framework of heavy-baryon χ PT: $0.0042(10) \text{ meV}$ [43] and $0.0029(12) \text{ meV}$ [44].

The above considerations take into account the most significant higher-order nucleon structure corrections that start to appear at N4LO in the $\not{\chi}$ EFT expansion. One can notice that each one of the corrections, $E_{2S}^{\text{hadr, FF}} = -0.013(1) \text{ meV}$ from Eq. (34), and the nucleon polarizability corrections, $E_{2S}^{\text{hadr, subt}} + E_{2S}^{\text{hadr, inel}} = -0.019(6) \text{ meV}$ from Eqs. (35) and (36), is separately smaller or of the size of the estimated

¹ Note that the leading pion-nucleon loop contribution to the subtraction-function correction was previously calculated with an approximate formula [39, Eq. (17a)] and has been updated here.

N3LO uncertainty of the inelastic contribution, 0.016 meV, Eq. (26). Their total, however,

$$E_{2S}^{\text{hadr}} = E_{2S}^{\text{hadr, FF}} + E_{2S}^{\text{hadr, subt}} + E_{2S}^{\text{hadr, inel}} = -0.032(6) \text{ meV}, \tag{37}$$

is about twice as large as that uncertainty. Nevertheless, we expect the higher-order nuclear effects, as well as the relativistic corrections, to be much smaller, and we expect the remaining higher-order effects to be within our N3LO uncertainty estimate. Erring on the side of caution, we refrain from going as far as performing an N4LO adjustment of the uncertainty.

3.4 Summary of results

We conclude this section by summarizing our $\not\pi$ EFT predictions of the nuclear-structure effects on the 2S level in μ D from the forward 2γ exchange, and including the accompanying electronic VP contributions. At N3LO, we derived the dominant 2γ -exchange effects coming from the elastic deuteron charge FF G_C and the non-pole part of the deuteron VVCS amplitude:

$$E_{2S}^{\text{elastic}} = -0.446(8) \text{ meV}, \tag{38a}$$

$$E_{2S}^{\text{inel}} = -1.509(16) \text{ meV}, \tag{38b}$$

see Sects. 3.1 and 3.2 for details. The uncertainties have been quantified through the Bayesian error estimate described in Appendix A. As mentioned above, the value of E_{2S}^{inel} contains the transverse contribution.

In Fig. 3, our $\not\pi$ EFT predictions are compared to data-driven and χ ET results. The disagreement with Carlson et al. [24] for E_{2S}^{elastic} is due to the deuteron charge FF parametrisation from Ref. [28]. As one can see from Table 2, our prediction is in good agreement with the data-driven approach if the Sick & Trautmann parametrisation [9] is used instead.

Beyond N3LO, we also take into account the single-nucleon effects discussed in Sect. 3.3. They can be split into the nucleon-polarizability contribution, the single-nucleon subtraction-function contribution, and the insertion of the nucleon FFs in the nucleon charge operator vertex of $\not\pi$ EFT. In total, they amount to:

$$E_{2S}^{\text{hadr}} = -0.032(6) \text{ meV}. \tag{39}$$

On top of the above forward 2γ -exchange effects,

$$E_{2S}^{\text{fwd}} = E_{2S}^{\text{elastic}} + E_{2S}^{\text{inel}} + E_{2S}^{\text{hadr}} = -1.987(20) \text{ meV}, \tag{40}$$

there are the electronic VP corrections to the 2γ -exchange, described in Appendix C:

$$E_{2S}^{\text{eVP}} = -0.027 \text{ meV} \tag{41}$$

(their uncertainty also being negligibly small). In total this adds up to:

$$E_{2S}^{\text{fwd+eVP}} = E_{2S}^{\text{fwd}} + E_{2S}^{\text{eVP}} = -2.014(20) \text{ meV}. \tag{42}$$

In Sect. 5, we will discuss all the relevant deuteron-structure effects, including also the Coulomb distortion from the off-forward 2γ exchange [5] and the 3γ -exchange effect [7].

4 Hydrogen–deuterium isotope shift

In this section, we will use the isotope shift between 1S and 2S states in H and D:

$$E_{\text{iso}} = h f_{\text{iso}} = E_{2S-1S}^{\text{D}} - E_{2S-1S}^{\text{H}}, \tag{43}$$

where h is the Planck constant, to get a prediction for the deuteron charge radius, cf. Eq. (2), and, in turn, determine the LEC l_1^{C0s} as given by Eq. (17). The empirically measured value of the isotope shift is very precise [45],

$$f_{\text{iso}} = 670\,994\,334.605(15) \text{ kHz}. \tag{44}$$

To extract from it r_d and l_1^{C0s} , we will update the theoretical prediction for the isotope shift. Our notation generally follows the work of Jentschura et al. [45]. It is, along with most of the features of the consideration in this section, such as a list of all contributions relevant to the isotope shift, presented in Appendix D. Here, we focus on our $\not\pi$ EFT result for the 2γ -exchange correction to the S-levels in D. The pertinent calculation proceeds analogously to Sect. 3, where the 2γ exchange in μ D is evaluated, hence its details are largely omitted.

4.1 2γ exchange in deuterium

The longitudinal part of the inelastic contribution to the 2S–1S shift in D is:

$$v_{9,L}^{\text{D}} = \left[16.612 - 0.769 l_1^{C0s} \right] \text{ kHz} \tag{45a}$$

$$= [9.929 + 6.825 - 0.062 - 0.078] \text{ kHz} = 16.613(191) \text{ kHz}. \tag{45b}$$

In the second line, we show our numerical order-by-order result with the LEC l_1^{C0s} determined in the following Sect. 4.2. Note that all forward 2γ -exchange contributions scale through the atomic wave function at the origin as $1/n^3$. Thus, to deduce the shift of the n^{th} S-level in D, one simply has to multiply the isotope shift value by $-8/7n^3$. The uncertainty of our result is obtained in a simplified way by multiplying the total by $(\gamma/m\pi)^4$. This is justified by the smallness of the N2LO and N3LO contributions (with the NLO contribution given by $(Z - 1)$ times the LO result plus a small correction, cf. Table 1 for the case of μ D).

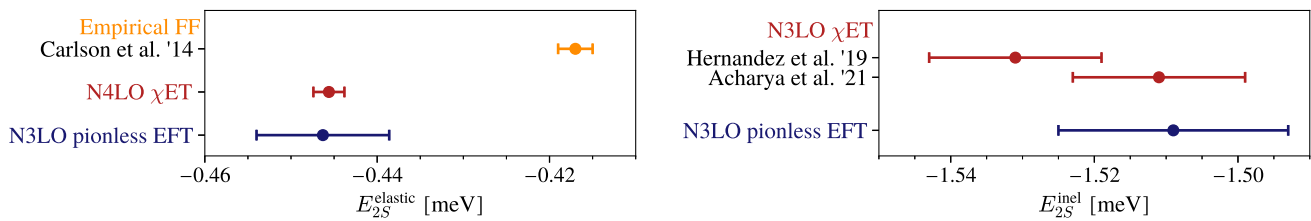


Fig. 3 Comparison of predictions for the elastic and inelastic contributions to the 2γ exchange in μD . Values are the same as in Tables 2 and 4

The transverse 2γ -exchange contribution appears to be relatively more important in D than in μD :

$$\Delta v_{9,T}^D = 1.859(65) \text{ kHz.} \tag{46}$$

The uncertainty is obtained here by multiplying the total with $(\gamma/m_\pi)^3$, where the usual NLO factor of $(\gamma/m_\pi)^2$ is multiplied with another γ/m_π to take into account that the transverse amplitude is well reproduced already at NLO [21, Sec. V]. The full N3LO $\not\pi$ EFT prediction for the inelastic contribution to the forward 2γ exchange is then given by

$$\Delta v_{9,L+T}^D = 18.472(202) \text{ kHz.} \tag{47}$$

The hadronic contributions to the shift of levels in D are as follows. Inserting the nucleon FFs as in Eq. (30) leads to a negligible shift:

$$\Delta v_{9, \text{hadr. FF}}^D = 0.014(1) \text{ kHz.} \tag{48}$$

The inelastic part, calculated in the same way as done for μD [24], gives [46]

$$\Delta v_{9, \text{hadr. inel}}^D = 0.148(11) \text{ kHz.} \tag{49}$$

This is in perfect agreement with the result from rescaling the single-nucleon values obtained in Ref. [41]: $\Delta v_{9, \text{hadr. inel}}^D = 0.145(12) \text{ kHz}$. The subtraction part is calculated by us in the same way as done for μD by rescaling the single-nucleon values from χ PT:

$$\Delta v_{9, \text{hadr. subt}}^D = -0.069(29) \text{ kHz.} \tag{50}$$

The subtraction function contributions found in Ref. [41] tend to be smaller, cf. Table 6.

The off-forward 2γ -exchange correction, known as the Coulomb distortion, can be estimated by rescaling the results for μD presented in Ref. [47]. For the $2S-1S$ shift in D, we obtain a very small result of $\simeq -0.034 \text{ kHz}$. Adding all contributions together, we find

$$\Delta v_9^D = [18.530 - 0.769 l_1^{C0s}] \text{ kHz} = 18.531(204) \text{ kHz.} \tag{51}$$

Table 6 Single-nucleon subtraction-function contributions from 2γ exchange between electron and proton (H) or neutron (en), respectively. The last column gives the $\Delta v_{9, \text{hadr. subt}}$ contribution to D, obtained by rescaling the electron–nucleon values. Values are in kHz

	H	en	D
χ PT [39,40]	-0.032(15)	-0.037(14)	-0.069(29)
data-driven	-0.016(4) [41]	-0.025(9) [41]	-0.041(13)

This has to be compared to $\Delta v_9^D = 18.70(7) \text{ kHz}$ used in Ref. [48] and based on Ref. [49].

The N3LO $\not\pi$ EFT prediction for the elastic contribution to the $2S-1S$ shift in D is

$$\Delta v_{(b)}^D = [0.625 + 1.607 l_1^{C0s}] \text{ kHz} \tag{52a}$$

$$= [0.292 + 0.221 + 0.087 + 0.023] \text{ kHz} \\ = 0.622(7) \text{ kHz,} \tag{52b}$$

where the uncertainty is estimated as above for $\Delta v_{9,L}^D$. This is slightly bigger than the pure Friar-radius contribution appearing in Ref. [48], which gives $\Delta v_{(b)}^D = 0.507 \text{ kHz}$.

Adding all 2γ -exchange corrections to the $2S-1S$ transition in D together, we find

$$\Delta v_{9+(b)}^D = [19.155 + 0.838 l_1^{C0s}] \text{ kHz} \\ = 19.153(204) \text{ kHz.} \tag{53}$$

One can see that the elastic and inelastic contributions proportional to l_1^{C0s} partially cancel each other, making the total slightly less sensitive to the value of the N3LO contact term, similarly to what happens in μD . In any case, the effect of it (assuming the maximal magnitude of $l_1^{C0s} \simeq 10^{-2}$) is at most 0.01 kHz, which is far smaller than the total uncertainty of the isotope shift. Therefore, the contribution of l_1^{C0s} to the 2γ exchange in the isotope shift can be safely neglected (at the current level of precision), and the deuteron charge radius extracted from the isotope shift is a good quantity to determine l_1^{C0s} .

4.2 2γ exchange in isotope shift and determination of low-energy constant l_1^{C0s}

For the isotope shift, we also need the 2γ -exchange correction to the $2S-1S$ transition in H. For the elastic contribution, we use the results from Ref. [41]:

$$\Delta v_{(b)}^H = 0.035(6) \text{ kHz}, \tag{54}$$

which is in perfect agreement with the Friar-radius contribution $\Delta v_{(b)}^H = 0.035 \text{ kHz}$ appearing in Ref. [48]. For the inelastic contribution, it is important that Δv_9^H is consistent with the single-proton contributions entering D through $\Delta v_9, \text{ hadr. inel}$ and $\Delta v_9, \text{ hadr. subt}$. Therefore, we will use the subtraction-function contribution predicted by χ PT, see Table 6, and the inelastic contributions from Ref. [41]:

$$\Delta v_9^H = [-0.032(15) + 0.073(5)] \text{ kHz} = 0.041(16) \text{ kHz}. \tag{55}$$

This compares to $\Delta v_9^H = 0.061(11) \text{ kHz}$ used in Ref. [48] and based on Ref. [50]. Using instead the subtraction-function contribution from Ref. [41], we would find:

$$\Delta v_9^H = 0.057(6) \text{ kHz}. \tag{56}$$

In total, the 2γ -exchange correction to the $2S-1S$ transition in H amounts to

$$\Delta v_{9+(b)}^H = 0.076(17) \text{ kHz}. \tag{57}$$

The combined results for the isotope shift are given in Eqs. (D19) and (D23) of Appendix D.

In the appendix, we give a full updated list of all contributions entering the isotope shift, together with a comparison to the values used in Ref. [45]. Besides theoretical updates, e.g., of the VP and recoil contributions, we discuss the impact of refined values for the electron, proton and deuteron masses, and the role of the Rydberg constant. Our final result for the theoretical prediction of the $2S-1S$ deuterium-hydrogen isotope shift reads:

$$f_{\text{iso}} = \left[671\,000\,534.811(924) + 0.838 l_1^{C0s} - 1369.346 \left(\frac{r_d}{\text{fm}}\right)^2 \right] \text{ kHz}. \tag{58}$$

Note that, in the calculation of the 2γ -exchange corrections, we used the value of the proton charge radius $r_p(\mu\text{H})$ published by the CREMA Collaboration, Eq. (1a). This value is consistent with the nucleon FF parametrisations from Ref. [35], used in Sect. 3.3 to estimate the single-nucleon effects beyond N3LO in $\not\chi$ EFT. The proton finite-size corrections to the isotope shift use instead a refined value [51], extracted from the Lamb shift measurement of the CREMA Collaboration [1,2] accounting for the recent updates of the μH theory [52–55]:

$$r_p(\mu\text{H}) = 0.84099(36) \text{ fm}. \tag{59}$$

The effect of the updated r_p value on the 2γ -exchange corrections would be negligibly small compared to the estimated theoretical uncertainties of the latter.

The LEC l_1^{C0s} is small (again, a reasonable estimate of its maximal magnitude being $\simeq 10^{-2}$). It is therefore justified to use the N3LO $\not\chi$ EFT prediction for the deuteron radius, given in Eq. (15), as an exact relation to express l_1^{C0s} in Eq. (58) through r_d . We can then extract r_d by comparing our theory prediction and the experimental value for the isotope shift (44):

$$r_d(\mu\text{H} \ \& \ \text{iso}) = 2.12788(16) \text{ fm}, \tag{60}$$

where the error is completely dominated by the theory. Our result for r_d is in perfect agreement with the previous extraction in Eq. (2). Setting $l_1^{C0s} = 0$ in Eq. (58) leads to the same result, which proves that the error generated by applying Eq. (15) as an exact relation can indeed be safely neglected. A comparison and consistency check of state-of-the-art deuteron charge radius extractions from μD , D and the H–D isotope shift can be found in Sect. 6.1. From Eq. (15), we then find:

$$l_1^{C0s} = -1.80(4)(36)(12) \times 10^{-3}, \tag{61}$$

where the uncertainties in the brackets stem from our extracted value of the deuteron radius, the uncertainty of $Z = 1.6893(30)$ [56], and the isoscalar nucleon charge radius $r_0 = 0.5586(10) \text{ fm}$, respectively.

5 Muonic deuterium Lamb shift

In this section, we will extract an empirical value for the 2γ -exchange effects in the μD Lamb shift from the high-precision Lamb shift measurement by the CREMA Collaboration [3] and the deuteron radius determined from the H–D isotope shift. The empirical value will be compared to our $\not\chi$ EFT prediction. A theory compilation for the μD spectrum, including a review of recent theoretical predictions for the 2γ -exchange effects, can be found in Ref. [5]. At the end of this section, we will present an updated theory prediction of the μD Lamb shift, based on our $\not\chi$ EFT prediction for the 2γ exchange, taking into account all recent theory improvements since the publication of Ref. [5].

5.1 Empirical 2γ exchange

The theory prediction for the μD Lamb shift reads [5, Eq. (18)]:

$$E_{2P-2S} = \left[228.77356(75) + 0.00310(60) \right]$$

$$-6.11025(28) \left(\frac{r_d}{\text{fm}} \right)^2 - E_{2S}^{2\gamma} \Big] \text{meV}. \tag{62}$$

Here, the first term is deuteron-radius independent, the next two terms are deuteron-radius dependent, and the last term contains deuteron-structure effects from 2γ exchange. Note that the prefactor in front of the radius-dependent finite-size term also contains radiative corrections, such as the electronic VP corrections partially discussed in Appendix C, see Ref. [5] for details.² The empirical value measured by the CREMA collaboration is:

$$E_{2P-2S} = 202.8785(31)_{\text{stat}}(14)_{\text{syst}} \text{meV}. \tag{63}$$

With the theory prediction for the Lamb shift in Eq. (62), the empirical value in Eq. (63), and $r_d(\mu\text{H} \ \& \ \text{iso})$ from Eq. (2), one obtains an empirical value for the 2γ -exchange effects in the μD Lamb shift [3]:

$$E_{2S}^{2\gamma}(\text{emp.}) = -1.7638(68) \text{meV}. \tag{64}$$

In the following, we update this value based on the improved hadronic VP [55] and electronic light-by-light scattering contributions [57], as well as $r_d(\mu\text{H} \ \& \ \text{iso})$ from Eq. (60).

For the effect of LO and NLO hadronic VP [55], combined with the mixed electronic and muonic VP, as well as the electronic VP loop in the SE correction [52], we use $(2P - 2S)$: $11.64(32) \ \mu\text{eV}$. This reduces the uncertainty of the old value $11.12(71) \ \mu\text{eV}$ (sum of # #12, 13, 14, 30, 31 in Ref. [5, Table 1]), thereby improving the uncertainty of the deuteron-radius independent term by a factor 2. In addition, we include the inelastic 3γ -exchange, calculated for the first time in Ref. [7]. Compared to Eq. (62), the elastic 3γ -exchange contribution (# #r3, r3' in [5, Table 2]) has been removed from the radius-dependent term, so that the sum of elastic and inelastic 3γ -exchange $(2P - 2S)$: $2.19(88)(27) \ \mu\text{eV}$ [7], is now listed as an individual term. The updated theory prediction for the Lamb shift in μD then reads [51]:

$$E_{2P-2S} = \left[228.77408(38) - 6.10801(28) \left(\frac{r_d}{\text{fm}} \right)^2 - E_{2S}^{2\gamma} + 0.00219(92) \right] \text{meV}. \tag{65}$$

Inserting the deuteron charge radius determined from the H–D isotope shift, Eq. (60), and comparing to the CREMA measurement, Eq. (63), we refine the empirical 2γ -exchange effect:

$$E_{2S}^{2\gamma}(\text{emp.}) = -1.7585(56) \text{meV}. \tag{66}$$

5.2 Comparison of theoretical predictions for 2γ exchange

² Note that in the final sum of radius-dependent terms in Ref. [5, Table 2] the entry #r8 has been included with a wrong sign.

Table 7 Comparison of prediction for the 2γ -exchange effects in the μD Lamb shift

	$E_{2S}^{2\gamma}$ [meV]
Theory prediction	
Krauth et al. [5]	-1.7096(200)
Kalinowski [6, Eq. (6) + (19)]	-1.740(21)
$\not\epsilon$ EFT N3LO	-1.752(20)
Empirical ($\mu\text{H} + \text{iso}$)	
Pohl et al. [3]	-1.7638(68)
This work	-1.7585(56)

In Sect. 3.4, we summarized our $\not\epsilon$ EFT results for the deuteron-structure effects in the μD Lamb shift originating from the forward 2γ exchange, including the accompanied electronic VP contributions, and compared to other theory predictions. Our final result is given in Eq. (42). For a meaningful comparison to the empirical value for the 2γ -exchange effect, Eq. (66), we need to add effects from off-forward 2γ exchange (the Coulomb distortions). Formally of a subleading $O(\alpha^6 \ln \alpha)$, they are, however, numerically important. We use the recommended value from the theory compilation in Ref. [5]:

$$E_{2S}^{\text{Coulomb}} = 0.2625(15) \text{meV}, \tag{67}$$

derived from modern deuteron potentials (χ ET potential and AV18 model [58]). This value should be consistent with the $\not\epsilon$ EFT framework, since the deuteron electric dipole polarizability from $\not\epsilon$ EFT [21] is in agreement with predictions from the applied deuteron potentials [59]. Combining Eqs. (42) and (67), our final result for the 2γ -exchange structure effects on the $2S$ -level in μD reads:

$$E_{2S}^{2\gamma} = -1.752(20) \text{meV}, \tag{68}$$

which is larger than the value accounted for in Ref. [5, Eq. (17)], but agrees with Ref. [6] within errors, cf. Table 7. It is also in agreement with the empirical value, Eq. (66), but more than a factor 3 less precise. Our new theory compilation will be used in Sect. 6.1 to extract $r_d(\mu\text{D})$ from the experimental value for E_{2P-2S} .

6 Charge radius extractions

6.1 Deuteron charge radius

This section compares three independent extractions of the deuteron charge radius: from the spectroscopy of the μD Lamb shift, the $2S-1S$ transition in D and the $2S-1S$ H–D isotope shift, respectively. With the experimental value

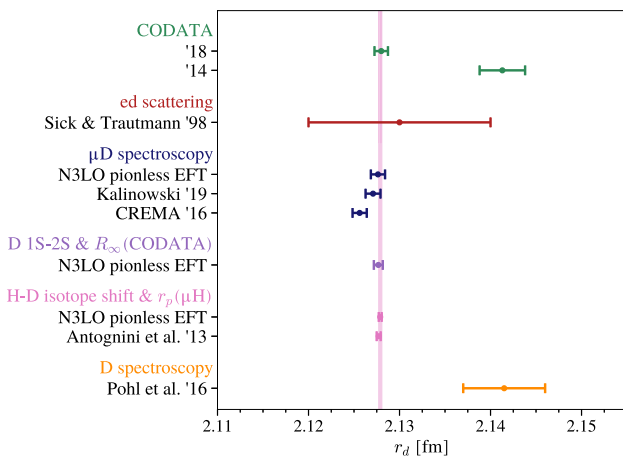


Fig. 4 Comparison of deuteron charge radius determinations from fits to electron–deuteron scattering data, ordinary and muonic-deuterium spectroscopy, and the 2S–1S hydrogen–deuterium isotope shift combined with the proton radius from muonic hydrogen

for the μD Lamb shift in Eq. (63), the theoretical prediction in Eq. (65), and our result for the 2γ -exchange effects, Eq. (68), we can extract the deuteron charge radius from μD spectroscopy:

$$r_d(\mu\text{D}) = 2.12763(13)_{\text{exp}}(77)_{\text{theory}} = 2.12763(78) \text{ fm}, \tag{69}$$

where the uncertainty budget remained the same as in the original extraction from Ref. [3], see Eq. (1b). In addition, we consider the extraction from the measured 2S–1S transition in D [60]:

$$f_{2S-1S}^{\text{D}} = 2\,466\,732\,407\,522.88(91) \text{ kHz}, \tag{70}$$

and the theory prediction in Eq. (F2), which leads to:

$$r_d(\text{D}, 2S-1S) = 2.12767(49) \text{ fm}. \tag{71}$$

Note that the entering Rydberg constant, R_∞ in Eq. (E4), is strongly driven by $r_p(\mu\text{H})$. The third extraction from the H–D isotope shift and $r_p(\mu\text{H})$ has been presented in Sect. 4.2:

$$r_d(\mu\text{H} \ \& \ \text{iso}) = 2.12788(16) \text{ fm}.$$

All results are shown in Fig. 4, together with older extractions, results from electron–deuteron scattering and the CODATA recommended values. We can see that the spectroscopy of ordinary and muonic hydrogen isotopes, after the recent theory updates, cf. Ref. [6], gives consistent results for the deuteron charge radius.

6.2 Proton charge radius

Analogously to the calculation of $r_d(\mu\text{H} \ \& \ \text{iso})$, we can use the isotope shift and $r_d(\mu\text{D})$ to extract the proton charge

radius:

$$r_p(\mu\text{D} \ \& \ \text{iso}) = 0.8404(20) \text{ fm}. \tag{72}$$

While a previous extraction along these lines, $r_p(\mu\text{D} \ \& \ \text{iso}) = 0.8356(20) \text{ fm}$ [3], had been in tension with $r_p(\mu\text{H})$, the result presented here based on the state-of-the-art theory predictions agrees. This, again, nicely shows the consistency between the spectroscopic analyses of ordinary and muonic hydrogen isotopes.

6.3 Proton–deuteron squared charge radii difference

Assuming $m_e \ll M_p \sim M_d$, we can find an approximation for the nuclear-size correction to the H–D isotope shift, Eq. (D22), which is related to the often quoted difference of squared proton and deuteron charge radii. The best such approximation turns out to be

$$\Delta f_{\text{iv}} \approx -\frac{7}{24\pi} \frac{\alpha^4 m_e^3 c^4}{\hbar^3 (1 + m_e/M_p)} [r_d^2 - r_p^2]. \tag{73}$$

We give here the charge radius difference exactly, based on Eqs. (59) and (60), and use the relation in Eq. (73) only to estimate the uncertainty, which is dominated by the theory of the isotope shift:

$$r_d^2 - r_p^2 = 3.820\,61(31) \text{ fm}^2. \tag{74}$$

Using Eq. (73) instead, the central value would decrease by about 1.5σ : $3.820\,13 \left(\begin{smallmatrix} +78 \\ -31 \end{smallmatrix} \right) \text{ fm}^2$. These results are in good agreement with the difference between charge radii extracted from the Lamb shift in muonic hydrogen isotopes:

$$r_d^2(\mu\text{D}) - r_p^2(\mu\text{H}) = 3.819\,55(337) \text{ fm}^2. \tag{75}$$

From Eq. (74), we can see that the larger CODATA '14 recommended value for the proton charge radius, $r_p = 0.8751(61) \text{ fm}$ [10], would impose a larger value for the deuteron radius inconsistent with the μD Lamb shift.

7 Conclusion and outlook

In this work, we calculated the 2γ -exchange corrections to the S-levels in ordinary and muonic deuterium in the $\not\pi$ EFT framework. The calculation was performed at N3LO, with the only unknown LEC I_1^{C0S} appearing at this order extracted using the H–D isotope shift, where the correlation between that LEC and the 2γ -exchange correction is negligible. In addition, we evaluated the contribution of the nucleon structure, i.e., the effect of the nucleon polarizability and of the shape of the nucleon FFs, which are the most important single-nucleon effects beyond N3LO. We also included the accompanying electronic vacuum polarization contributions.

Our predictions for the elastic contribution to the 2γ exchange in μD from $\not\{EFT}$ at N3LO and χET at N4LO appear to be several standard deviations larger than the evaluations [24, 29] based on the deuteron charge FF parametrisation of Ref. [28], cf. Fig. 3 and Table 2. This suggests that the latter parametrisation does not adequately describe the behaviour of the deuteron charge FF at low virtualities. The correlation between the Friar radius r_{Fd} and the deuteron charge radius r_d in $\not\{EFT}$, cf. Fig. 2, through the LEC l_1^{C0s} could serve as a diagnostic criterion for a realistic parametrisation of the deuteron charge FF. We also point out that the $\not\{EFT}$ expression for the deuteron charge FF at N3LO [21, Sec. IV] can be used for an analytic one-parameter fit to the electron–deuteron scattering data in the low- Q^2 range relevant to the planned DRad experiment [31].

Supplementing the μD theory [5] with a few missing electronic VP effects [6] and the inelastic 3γ exchange [7], together with the shift of the elastic contribution found in this work, the past discrepancy between theory and experiment on the size of 2γ -exchange effects, see Table 7, is now completely resolved.

The uncertainty of the theoretical result for the 2γ -exchange correction was quantified using Bayesian inference. While our N3LO $\not\{EFT}$ prediction was not yet able to improve the theoretical precision, the improved understanding of the elastic contribution is of utmost importance. In addition, by calculating the 2γ -exchange correction to μD and D, we were able to perform a few consistency checks. In particular, we showed that extractions of the deuteron charge radius from the μD Lamb shift, the $2S-1S$ transition in D and the $2S-1S$ H–D isotope shift, cf. Fig. 4, are now in excellent agreement.

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Appendix A: Quantification of uncertainty

The uncertainty of an EFT calculation is in many cases, including the present work, dominated by the unknown higher-order terms rather than input parameters. To quantify the uncertainty, we follow the Bayesian approach developed in Refs. [20, 63] and references therein. The results and the details specific to our evaluation are presented in this section.

We start with the EFT expansion of a generic observable A in powers of the expansion parameter ξ (which is $\xi = \gamma/m_\pi$ in $\not\{EFT}$):

$$A = A_0 \sum_{n=0}^{\infty} c_n \xi^n, \quad (\text{A1})$$

where the parameter A_0 sets the scale of A , and c_n are the expansion coefficients. The uncertainty of A caused by a truncation at $n = k$ is given by the unknown remainder:

$$\Theta A_k = A_0 \sum_{n=k+1}^{\infty} c_n \xi^n. \quad (\text{A2})$$

The typical prior assumption used in EFT calculations is the naturalness of the expansion coefficients, i.e., c_n should be at most $O(1)$. One may refine this assumption using the calculated expansion coefficients as done in, e.g., Ref. [64] that assigns (written out here for an N3LO calculation, $k = 3$):

$$\begin{aligned} \Theta A_3 &= \max \left\{ \xi^4 |\Delta A^{\text{LO}}|, \xi^3 |\Delta A^{\text{NLO}}|, \xi^2 |\Delta A^{\text{N2LO}}|, \right. \\ &\quad \left. \xi |\Delta A^{\text{N3LO}}| \right\} \\ &= A_0 \xi^4 \max_{n \leq 3} |c_n|, \end{aligned} \quad (\text{A3})$$

where ΔA^{LO} , ΔA^{NLO} , etc. are the contributions to A at the respective order. This also implicitly assumes that ΘA_k is dominated by its first term, $A_0 c_{k+1} \xi^{k+1}$; we will employ this assumption in the following (note that it can be relaxed, in particular, in the Bayesian approach [20, 63]). Looking at the expansion of E_{2S} , we note that the expansion of the LSZ factor, $[\Sigma'(E_d)]^{-1} \propto 1 + (Z - 1) + 0 + 0 + \dots$, see Ref.

[21, Eq. (49)], results in every term appearing at a given order in the four-point function acquiring a factor of Z at the next order, as is also explicitly shown in Table 1. This induces correlations between the coefficients in the expansion. It is therefore natural to slightly modify the expansion for the purpose of quantifying the uncertainty, taking out the known Z factor along with the scale factor A_0 . This amounts to working with the expansion of the (integrals of) the four-point functions, and the simple estimate of Eq. (A3) becomes:

$$\Theta A_3 = Z A_0 \xi^4 \max_{n \leq 3} |c_n|, \tag{A4}$$

where A_0 and c_n are now the normalization and the expansion coefficients of the integrals of the four-point function, which can be deduced from Table 1, respectively, for E_{2S}^{elastic} and $E_{2S}^{\text{inel},L}$.

Moving to the Bayesian quantification, we use the prior probability density functions (PDFs) introduced in Ref. [20] as Sets A, B, and C. Each one of the sets of priors consists of two PDFs, $\text{pr}(c)$ and $\text{pr}(c_n|c)$, where the first is associated with the scale c typical of the coefficients c_n , while the second describes the probability distribution of c_n given the scale. In the leading-term approximation for the uncertainty, the Bayes' theorem with the given prior PDFs gives the PDF of the uncertainty at order k , given the known c_0, \dots, c_k :

$$\text{pr}(\Theta A_k | c_0, \dots, c_k) = \frac{\int_0^\infty dc \text{pr}(c_{k+1}|c) \text{pr}(c) \prod_{m=0}^k \text{pr}(c_m|c)}{Z A_0 \xi^{k+1} \int_0^\infty dc \text{pr}(c) \prod_{m=0}^k \text{pr}(c_m|c)} \tag{A5}$$

with

$$c_{k+1} = \frac{\Theta A_k}{Z A_0 \xi^{k+1}}, \tag{A6}$$

where we specialize to the case of E_{2S} and the quantities A_0 and c_n again pertain to the expansion of the (integrals of) the four-point function (with the Z factored out).

The expansion coefficients and prefactors that correspond to the modified $\not\pi$ EFT expansion of E_{2S}^{elastic} , $E_{2S}^{\text{inel},L}$, and their sum $E_{2S}^{\text{sum}} = E_{2S}^{\text{elastic}} + E_{2S}^{\text{inel},L}$, are given in Table 8. One can see that the expansion coefficients of the elastic contribution are somewhat larger than one, whereas the inelastic part, as well as the total, have smaller expansion coefficients. There are partial cancellations between the higher-order elastic and inelastic contributions, which, together with the LO total term being about five times larger than its elastic counterpart, suppresses the expansion coefficients of the total 2γ -exchange correction. With these coefficients, we start with the estimate of Eq. (A4), which gives:

$$\Theta \left(\left\{ E_{2S}^{\text{elastic}}, E_{2S}^{\text{inel},L}, E_{2S}^{\text{sum}} \right\} \right)$$

$$= \{0.009, 0.018, 0.022\} \text{ meV}. \tag{A7}$$

The uncertainties deduced this way are a priori not Gaussian-distributed quantities (as one sees explicitly from, e.g., the Bayesian PDFs below, cf. Fig. 5), therefore the usual addition of uncertainties in quadrature may not be an adequate way to, e.g., calculate the uncertainty of a sum given the uncertainties of its constituents; we therefore estimate the uncertainty of E_{2S}^{sum} independently.

Proceeding to the Bayesian estimates, we apply Eq. (A5) with the priors of Ref. [20] to the results of our calculation. The specific parameters that we use for the priors are:

$$c_> = 100, \quad c_< = 10^{-3}, \quad \sigma = 2.0. \tag{A8}$$

The resulting PDFs for ΘA_3 are shown in Fig. 5. Set A and Set B result in PDFs that in each case are practically on top of each other, we therefore show only Set A as a representative, along with Set C.

The Bayesian procedure results in the following 68% degree-of-belief (DOB) intervals:

$$\begin{aligned} \text{Set A : } \quad & \Theta \left(\left\{ E_{2S}^{\text{elastic}}, E_{2S}^{\text{inel},L}, E_{2S}^{\text{sum}} \right\} \right) \\ & = \{0.0078, 0.0156, 0.0189\} \text{ meV}, \end{aligned} \tag{A9a}$$

$$\begin{aligned} \text{Set B : } \quad & \Theta \left(\left\{ E_{2S}^{\text{elastic}}, E_{2S}^{\text{inel},L}, E_{2S}^{\text{sum}} \right\} \right) \\ & = \{0.0077, 0.0155, 0.0188\} \text{ meV}, \end{aligned} \tag{A9b}$$

$$\begin{aligned} \text{Set C : } \quad & \Theta \left(\left\{ E_{2S}^{\text{elastic}}, E_{2S}^{\text{inel},L}, E_{2S}^{\text{sum}} \right\} \right) \\ & = \{0.0071, 0.0111, 0.0133\} \text{ meV}. \end{aligned} \tag{A9c}$$

One can see that the simple estimate of Eq. (A7) gives a more conservative uncertainty than is obtained from the Bayesian framework, which was also the tendency observed in Ref. [20]. It is also evident that the priors Set A and B result in somewhat bigger uncertainties than Set C; the difference is rather small for the elastic contribution, but is of the order of 25% for the inelastic term and the total 2γ -exchange correction. Seeing that the current uncertainty estimate uses the leading omitted term approximation, one can expect an about 30% change in the uncertainty once higher-order terms are taken into account. The above difference between Sets A and B, on the one hand, and Set C, on the other hand, is thus not unexpectedly big. One can also note that the uncertainty of the elastic term is probably overestimated, since higher-order terms are unlikely to change that term as much as suggested by the projected uncertainty, given that the value of r_d^2 is fixed at N3LO. This is also supported by the agreement between the $\not\pi$ EFT and χ ET results for the elastic contribution. We take the more conservative results of Sets A and B as our uncertainty estimate for the calculated 2γ -exchange contributions.

Table 8 Expansion coefficients and prefactors corresponding to the modified $\not\epsilon$ EFT expansion

	A_0 [meV]	c_0	c_1	c_2	c_3
E_{2S}^{elastic}	-0.204	1	0.260	2.311	-1.896
$E_{2S}^{\text{inel},L}$	-0.943	1	-0.050	-0.379	0.044
E_{2S}^{sum}	-1.148	1	0.006	0.100	-0.301

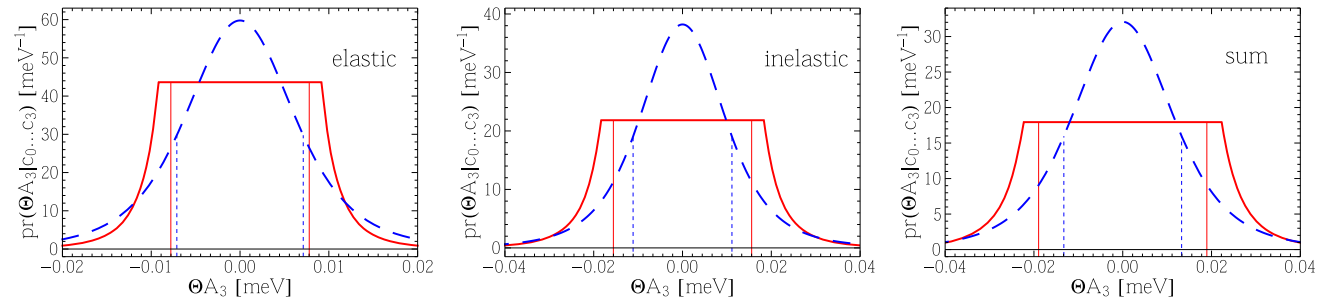


Fig. 5 Probability distribution functions for $\Theta(E_{2S}^{\text{elastic}})$ (left), $\Theta(E_{2S}^{\text{inel},L})$ (center), and $\Theta(E_{2S}^{\text{sum}})$ (right). Red solid (blue dashed) curves correspond to Set A (Set C) priors. Thin vertical lines indicate the corresponding 68% degree-of-belief intervals

Finally, one may notice that, in particular, the relative smallness of the higher-order coefficients in Table 8, might mean that the assignment $\xi = 1/3$ overestimates the size of the expansion parameter (and thus also the truncation uncertainty). As demonstrated in, e.g., Ref. [20] with χ ET calculations, Bayesian tools could also be applied to quantify the (assigned) value of the expansion parameter. Such a study would ideally involve additional quantities obtained in the same $\not\epsilon$ EFT framework, and will be presented elsewhere; in this context, see Ref. [65] that studies the uncertainties arising from a different expansion employed in calculations of 2γ -exchange corrections in muonic atoms and ions.

Appendix B: Deuteron VVCS amplitudes with insertion of nucleon form factors

In this appendix, we provide the expressions for the longitudinal deuteron VVCS amplitude at LO and NLO resulting from the procedure outlined in Sect. 3.3, where one inserts the full nucleon FFs. The expressions for the four-point function (see Ref. [21, Sec. II D] for the definition) with the inserted FFs read:

$$\begin{aligned} \mathcal{M}_L^{(-3), \text{FF}} = & \frac{e^2 M^3 Q^2}{\pi q^2} \left\{ \frac{[\bar{G}_E^0(Q^2)]^2 + [\bar{G}_E^1(Q^2)]^2}{\gamma [q^2 + 4(\gamma + \lambda_d)^2]} \right. \\ & + \frac{[\bar{G}_E^0(Q^2)]^2 - [\bar{G}_E^1(Q^2)]^2}{M|q|\nu} \phi(\nu, q^2) \\ & \left. - \frac{4[\bar{G}_E^0(Q^2)]^2}{q^2(\gamma - \lambda_d)} \phi^2(\nu, q^2) \right\} \\ & + (\nu \rightarrow -\nu), \end{aligned} \tag{B1}$$

$$\begin{aligned} \mathcal{M}_L^{(-2), \text{FF}} = & \frac{e^2 M^3 Q^2}{\pi q^2} \frac{2(Z-1)}{\gamma} [\bar{G}_E^0(Q^2)]^2 \\ & \times \frac{\phi(\nu, q^2) [|\mathbf{q}| - (\gamma + \lambda_d)\phi(\nu, q^2)]}{q^2(\gamma - \lambda_d)} \\ & + (\nu \rightarrow -\nu). \end{aligned} \tag{B2}$$

Here, the kinematic functions are [21]:

$$\lambda_d = \sqrt{\gamma^2 - M\nu + \frac{q^2}{4}}, \quad \phi(\nu, q^2) = \arctan \frac{|\mathbf{q}|}{2(\gamma + \lambda_d)}, \tag{B3}$$

and the barred nucleon isoscalar and isovector electric FFs are:

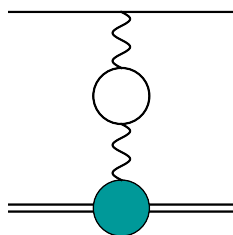
$$\bar{G}_E^{0,1}(Q^2) = \frac{G_E^{0,1}(Q^2)}{\sqrt{1 + \frac{Q^2}{4M_p^2}}}. \tag{B4}$$

Appendix C: Electronic vacuum polarization corrections to finite-size and polarizability contributions

In this appendix, we consider the one-loop electronic VP given by:

$$\begin{aligned} \bar{\Pi}^{(1)}(Q^2) = & \Pi^{(1)}(Q^2) - \Pi^{(1)}(0) \\ = & \frac{\alpha}{3\pi} \left[2 \left(1 - \frac{1}{2\tau_e} \right) \right. \\ & \left. \times \left(\sqrt{1 + \frac{1}{\tau_e}} \operatorname{arccoth} \sqrt{1 + \frac{1}{\tau_e}} - 1 \right) + \frac{1}{3} \right], \end{aligned} \tag{C1}$$

Fig. 6 One-photon exchange with vacuum-polarization and finite-size correction



with $\tau_e = Q^2/4m_e^2$ and m_e the electron mass, and its well known corrections to the deuteron structure effects.

We start with the corrections to the $O(\alpha^4)$ deuteron radius term to illustrate the approach, before calculating the corrections to the $O(\alpha^5)$ 2γ -exchange effect, relevant for this paper. The one-loop electronic VP correction to the deuteron charge radius term, see Fig. 6, is described by the following potential:

$$\Delta V_{VP\text{-}FF}(r) = - \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi\alpha}{q^2} \bar{\Pi}^{(1)}(q^2) \times [G_C(q^2) - 1]. \tag{C2}$$

Note that this is a contribution to the Breit potential [66, Ch. IX, §83], where the retardation effects can be neglected at this order in α , and hence Q^2 is replaced by q^2 . We shall make use of the dispersion relations (DRs) for the VP and the FF:

$$\bar{\Pi}(Q^2) = -\frac{Q^2}{\pi} \int_{4m_e^2}^{\infty} dt \frac{\text{Im } \Pi(t)}{t(t + Q^2)}, \tag{C3a}$$

$$G_C(Q^2) = \frac{1}{\pi} \int_{t_0}^{\infty} dt' \frac{\text{Im } G_C(t')}{t' + Q^2}, \tag{C3b}$$

where f denotes the principal-value integration. The one-loop expression for the absorptive part of electronic VP reads:

$$\text{Im } \Pi^{(1)}(t) = -\frac{\alpha}{3} \left(1 + \frac{2m_e^2}{t}\right) \sqrt{1 - \frac{4m_e^2}{t}}. \tag{C4}$$

The DR for VP is once-subtracted to ensure the correct normalisation of the electromagnetic field. Similarly to ensure the correct normalisation of the deuteron charge, $G_C(0) = 1$, we can use the once-subtracted relation for the charge FF:

$$G_C(Q^2) - 1 = -\frac{Q^2}{\pi} \int_{t_0}^{\infty} dt' \frac{\text{Im } G_C(t')}{t'(t' + Q^2)}. \tag{C5}$$

In first-order perturbation theory to the unperturbed Coulomb wave functions, one finds for the Lamb shift:

$$E_{2P-2S}^{(1)(VP\text{-}FF)} = -\frac{\alpha^4 m_r^3}{2\pi} \left(\int_{4m_e^2}^{\infty} dt \frac{\text{Im } \Pi^{(1)}(t)}{(\sqrt{t} + \alpha m_r)^4} [G_C(t) - 1] + \int_{t_0}^{\infty} dt' \frac{\text{Im } G_C(t')}{(\sqrt{t'} + \alpha m_r)^4} \bar{\Pi}^{(1)}(t') \right). \tag{C6}$$

It is clear that the dominant effect comes from the small- t region in the first integral, which starts from the threshold of e^+e^- production. Unfortunately, we cannot simply expand

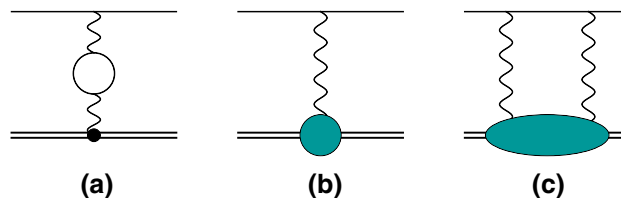


Fig. 7 **a** One-photon exchange with vacuum polarization; **b** one-photon exchange with finite-size correction; and **c** elastic and inelastic two-photon exchange

G_C around 0 before integration, since the integral will eventually diverge. Instead we use again the DR for G_C given in Eq. (C3a). We then change the variable $t \rightarrow 4m_e^2 u^2$ and perform the integration over u . Afterwards, only integrals over t' remain, which start from the threshold of hadron (e.g., $\pi^+\pi^-$) production t_0 . Assuming that $2m_e \ll t_0 \leq t'$, we can expand up to $O(4m_e^2/t')$. Neglecting terms which are suppressed by additional factors of m_e^2 , we obtain:

$$E_{2P-2S}^{(1)(VP\text{-}FF)} = -\frac{1}{6} \alpha^5 m_r^3 A(\kappa) r_d^2 \tag{C7a}$$

$$= -0.0135 \left[\frac{r_d}{\text{fm}} \right]^2 \text{ meV} \tag{C7b}$$

$$\simeq -0.06113(1) \text{ meV},$$

with the auxiliary function:

$$A(\kappa) = \frac{1}{12\pi(1 - \kappa^2)^2} \left[\kappa^2(4\kappa^2 - 7) + \frac{\kappa(4\kappa^4 - 10\kappa^2 + 9)}{\sqrt{1 - \kappa^2}} \arccos \kappa \right] \simeq 0.152309 \tag{C8}$$

at $\kappa = \alpha m_r / 2m_e$. Our formula agrees numerically with Ref. [67, Eq. (28)]. In Eq. (C7b), we used the deuteron radius determined through the isotope shift to illustrate the quantitative size of the effect, where the uncertainty is just propagated from the error of the radius in Eq. (60).

A similar subleading correction stems from the interference of one-photon exchange potentials with electronic VP,

$$\Delta V_{VP}(r) = - \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi\alpha}{q^2} \bar{\Pi}^{(1)}(q^2) = \frac{\alpha}{\pi} \int_{4m_e^2}^{\infty} dt \frac{\text{Im } \Pi^{(1)}(t)}{t} \frac{e^{-r\sqrt{t}}}{r}, \tag{C9}$$

and finite-size corrections,

$$\Delta V_{FF}(r) = - \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi\alpha}{q^2} [G_C(q^2) - 1] \simeq \frac{4\pi\alpha}{6} r_d^2 \delta(\mathbf{r}), \tag{C10}$$

see Fig. 7a, b, respectively. The latter can be approximated with a delta-function potential proportional to the deuteron radius. To calculate this effect at second order in perturbation theory, we need to know the matrix elements of the delta-function and Yukawa-type potentials between the μ D Coulomb wave functions:

$$\langle 2S|\delta(\mathbf{r})|nS\rangle = \frac{1}{2\sqrt{2n^3\pi a^3}}, \tag{C11a}$$

$$\begin{aligned} \langle 2S|e^{-r\sqrt{t}}/r|nS\rangle &= -\frac{4\sqrt{2n}}{a} \frac{4-n^2(3+4a^2t)}{[n^2(1+2a\sqrt{t})^2-4]^2} \\ &\times \exp\left[-2n \operatorname{arctanh} \frac{2}{n(1+2a\sqrt{t})}\right], \end{aligned} \tag{C11b}$$

and the energy levels of the Coulomb potential:

$$E_n = -\frac{\alpha}{2an^2}, \quad E_2 = -\frac{\alpha}{8a}, \tag{C12}$$

with n the principal quantum number. For the discrete spectrum, we obtain:

$$E_{2S}^{(2)\text{disc.}\langle\text{VP}\rangle\langle\text{FF}\rangle} = 2 \sum_{n \neq 2} \frac{\langle 2S|\Delta V_{\text{VP}}|nS\rangle \langle 2S|\Delta V_{\text{FF}}|nS\rangle}{E_2 - E_n} \tag{C13}$$

$$\begin{aligned} &\simeq \frac{4\alpha^2 r_d^2}{3} \sum_{n \neq 2} \frac{1}{E_2 - E_n} \langle 2S|\delta(\mathbf{r})|nS\rangle \\ &\times \int_{4m_e^2}^{\infty} dt \frac{\operatorname{Im} \Pi^{(1)}(t)}{t} \langle 2S|e^{-r\sqrt{t}}/r|nS\rangle \end{aligned} \tag{C14}$$

$$\begin{aligned} &= -0.008274 \left[\frac{r_d}{\text{fm}}\right]^2 \text{ meV} \\ &\simeq -0.037464(6) \text{ meV}, \end{aligned} \tag{C15}$$

with the deuteron radius in fm units. For the continuous spectrum, we apply:

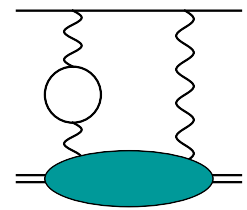
$$\langle 2S|\delta(\mathbf{r})|kS\rangle = \frac{1}{2\sqrt{2\pi a^3}} \sqrt{\frac{k}{1-e^{-2\pi/k}}}, \tag{C16a}$$

$$\begin{aligned} \langle 2S|e^{-r\sqrt{t}}/r|kS\rangle &= \frac{4\sqrt{2}}{a} \frac{3+4(a^2t+k^2)}{[4k^2+(1+2a\sqrt{t})^2]^2} \\ &\times \exp\left[-\frac{2}{k} \arctan \frac{2k}{1+2a\sqrt{t}}\right] \\ &\times \sqrt{\frac{k}{1-e^{-2\pi/k}}}, \end{aligned} \tag{C16b}$$

and

$$E_k = \frac{\alpha k^2}{2a}, \tag{C17}$$

Fig. 8 Elastic and inelastic two-photon exchange with vacuum-polarization insertion at $O(\alpha^6)$



to get:

$$E_{2S}^{(2)\text{cont.}\langle\text{VP}\rangle\langle\text{FF}\rangle} = 2 \int_0^{\infty} dk \frac{\langle 2S|\Delta V_{\text{VP}}|kS\rangle \langle 2S|\Delta V_{\text{FF}}|kS\rangle}{E_2 - E_k} \tag{C18}$$

$$\begin{aligned} &\simeq \frac{\sqrt{2}\alpha^2 r_d^2}{3\pi a^3} \int_0^{\infty} dk \sqrt{\frac{k}{1-e^{-2\pi/k}}} \frac{1}{E_2 - E_k} \\ &\times \int_{4m_e^2}^{\infty} dt \frac{\operatorname{Im} \Pi^{(1)}(t)}{t} \langle 2S|e^{-r\sqrt{t}}/r|kS\rangle \end{aligned} \tag{C19}$$

$$\begin{aligned} &= 0.028761 \left[\frac{r_d}{\text{fm}}\right]^2 \text{ meV} \\ &\simeq 0.130226(20) \text{ meV}. \end{aligned} \tag{C20}$$

In total, the interference of the one-photon-exchange potentials in Fig. 7a, b amounts to:

$$E_{2S}^{(2)\langle\text{VP}\rangle\langle\text{FF}\rangle} = E_{2S}^{(2)\text{disc.}\langle\text{VP}\rangle\langle\text{FF}\rangle} + E_{2S}^{(2)\text{cont.}\langle\text{VP}\rangle\langle\text{FF}\rangle} \tag{C21}$$

$$\begin{aligned} &= 0.020487 \left[\frac{r_d}{\text{fm}}\right]^2 \text{ meV} \\ &\simeq 0.092763(14) \text{ meV}. \end{aligned} \tag{C22}$$

This formula agrees numerically with Ref. [67, Eq. (29)].

Let us now turn to our main interest: the electronic VP corrections to the 2γ exchange. The simplest correction is due to the insertion of the one-loop electronic VP into the 2γ -exchange diagram, see Fig. 8. We multiply the integrand in Eq. (9a) with $[1 - \overline{\Pi}^{(1)}(Q^2)]^{-2}$ and obtain for the sum of elastic and inelastic contributions:

$$\begin{aligned} E_{2S}^{(1)\langle 2\gamma\text{-VP}\rangle} &= [-0.0071 - 0.0136] \text{ meV} \\ &= -0.0207 \text{ meV}. \end{aligned} \tag{C23}$$

In addition, there is a correction to the μ D atomic wave function that can be calculated at second order in perturbation theory from the interference of the one-photon exchange potential with VP insertion, Eq. (C9), and the forward 2γ -exchange potential:

$$\Delta V_{2\gamma}(r) = \frac{E_{nS}^{\text{fwd}}}{[\phi_n(0)]^2} \delta(\mathbf{r}), \tag{C24}$$

see Fig. 7a, c, respectively. Since the latter is a delta-function potential just like our approximated one-photon exchange

potential with finite-size correction, Eq. (C10), the calculation of $E_{2S}^{(2)(VP)(2\gamma)}$ proceeds analogously to the calculation of $E_{2S}^{(2)(VP)(FF)}$ above. We therefore present here only the results:

$$E_{2S}^{(2)disc.(VP)(2\gamma)} = 0.0013624 E_{2S}^{fwd} \simeq -0.00271 \text{ meV}, \tag{C25a}$$

$$E_{2S}^{(2)cont.(VP)(2\gamma)} = -0.0047358 E_{2S}^{fwd} \simeq 0.00941 \text{ meV}, \tag{C25b}$$

$$E_{2S}^{(2)(VP)(2\gamma)} = E_{2S}^{(2)disc.(VP)(2\gamma)} + E_{2S}^{(2)cont.(VP)(2\gamma)} \tag{C25c}$$

$$= 1.4523 \frac{\alpha}{\pi} E_{2S}^{fwd} = 0.0033734 E_{2S}^{fwd} = -0.00670(7) \text{ meV}. \tag{C25d}$$

The formula agrees numerically with the wave function correction in Refs. [6, Eqs. (17) and (18)] and [54, Table II]. Here we used the full forward 2γ -exchange result, $E_{2S}^{fwd} = -1.987(20) \text{ meV}$, collected in Eq. (40), and propagated its uncertainty into Eq. (C25d).

The sum of electronic VP corrections to the 2γ exchange, amounts to:

$$E_{2S}^{eVP} = E_{2S}^{(1)(2\gamma-Vp)} + E_{2S}^{(2)(VP)(2\gamma)} = -0.0274 \text{ meV}, \tag{C26}$$

which is about a factor one-and-a-half larger than our error estimate for E_{2S}^{fwd} . Our result is comparable to the results of Ref. [6, Eq. (19)]: $E_{2S}^{eVP} = -0.0265(3) \text{ meV}$.

Appendix D: Hydrogen–deuterium isotope shift

In this appendix, we will update the analysis of the H–D isotope shift presented in Ref. [45], which is based on the framework reviewed in the CODATA 2006 report [48]. More recent summaries of the theory of hydrogen-like atoms can be found, e.g., in Refs. [7,68]. The most relevant physical constants entering the isotope shift calculation are listed below, with their relative uncertainties given in square brackets:

$$\begin{aligned} m_e &= 9.109\,383\,7015(28) \times 10^{-31} \text{ kg} & [3.1 \times 10^{-10}], \\ \frac{m_e}{M_p} &= 5.446\,170\,214\,87(33) \times 10^{-4} & [6.0 \times 10^{-11}], \\ \frac{m_e}{M_d} &= 2.724\,437\,107\,462(96) \times 10^{-4} & [3.5 \times 10^{-11}], \\ \frac{M_d}{M_p} &= 1.999\,007\,501\,39(11) & [5.6 \times 10^{-11}], \\ \alpha^{-1} &= 137.035\,999\,084(21) & [1.5 \times 10^{-10}], \\ R_{\infty}c &= 3.289\,841\,960\,2508(64) \times 10^{15} \text{ Hz} & [1.9 \times 10^{-12}]. \end{aligned} \tag{D1}$$

The values are taken from the latest CODATA and PDG reports [4,69]. Compared to the CODATA 2006 report [48], the relative uncertainties have improved by a factor 3.5 to 12. The relative uncertainty of m_e has even shrunk by two orders of magnitude. The Rydberg constant, R_{∞} , listed above is a result of the CODATA 2018 fit of various measured transitions in hydrogen-like atoms. It is, however, largely driven by the Lamb shift in μH . A similar result is obtained relying solely on the Lamb shift in μH and the $2S-1S$ transition in H, see our determination in Appendix E.

In Ref. [45], the various contributions to the isotope shift are split into four Sets (i)–(iv). The bulk of the isotope shift comes from the respective difference of the Dirac eigenvalues once the reduced mass effects are accounted for, identified in Ref. [45] as Set (i). Based on the newest CODATA 2018 set of physical constants, we evaluate the frequency shift as:

$$\begin{aligned} \Delta f_i &= 671\,004\,071.028(85) \text{ kHz} \\ & [671\,004\,071.29(66) \text{ kHz}]. \end{aligned} \tag{D2}$$

This is 262 Hz smaller than the old value (given in square brackets) obtained using the CODATA 2006 set of constants, and considerably more precise. As mentioned already, the best values for the Rydberg constant, see Eqs. (D1) and (E4), are determined i.a. from the experimental $2S-1S$ transition in H, thus, rely on the same theory input as the $2S-1S$ H–D isotope shift. However, since they are largely driven by $r_p(\mu\text{H})$, it is justified to use these values in our analysis. Both central value and uncertainty estimate, following Ref. [45], are the same for Δf_i with Eqs. (D1) and (E4), respectively.

We should also mention that since the latest CODATA adjustment, there have been many advances in the experimental determination of the electron–proton mass ratio [70–72] and the proton–deuteron mass ratio [73,74]. The presently most precise values (relative uncertainty in square brackets),

$$\frac{m_e}{M_p} = 5.446\,170\,214\,805(98) \times 10^{-4} \quad [1.8 \times 10^{-11}],$$

$$\frac{M_d}{M_p} = 1.999\,007\,501\,243(31) \quad [1.6 \times 10^{-11}],$$

are based on an improved theory of rovibrational spin-averaged transitions in the hydrogen molecular ion HD^+ [75]. From this it also follows that:

$$\frac{m_e}{M_d} = 2.724\,437\,107\,624(65) \times 10^{-4} \quad [2.4 \times 10^{-11}].$$

Using these values to calculate the effect of the dominant Dirac eigenvalue contribution to the isotope shift, we obtain:

$$\Delta f_i = 671\,004\,070.972(29) \text{ kHz}, \tag{D3}$$

in agreement with Eq. (D2), but almost a factor three more precise. Note that the 5σ variance between the latest determi-

nation of the fine structure constant α from a rubidium recoil measurement [76] and the best caesium recoil measurement [77] has no effect on the isotope shift.

The next by size Set (ii) of Ref. [45] includes ten contributions with frequency shifts $\Delta\nu_j$. We checked that we reproduce the numbers for this set from Ref. [45] individually, using the constants and the formalism given in the CODATA 2006 report [48], up to 0.01 kHz. The new CODATA 2018 constants do not have a significant effect here. However, there have been considerable improvements of the theory, as we show in our updated evaluation below (old values in square brackets):

1. One-loop SE and electronic VP:

$$\Delta\nu_1 = -5558.999 \text{ kHz} \quad [-5558.99 \text{ kHz}]. \quad (\text{D4})$$

2. Two-loop SE, electronic VP, and combined effects:

$$\Delta\nu_2 = -0.521(1) \text{ kHz} \quad [-0.51 \text{ kHz}]. \quad (\text{D5})$$

Here, we use updated values for the coefficients [10]:

$$B_{50}(nS) = -21.55447(13) \quad [-21.5561(31)], \quad (\text{D6})$$

$$B_{60}(1S) = -81.3(0.3)(19.7) \quad [-95.3(0.3)(33.7)], \quad (\text{D7})$$

$$B_{60}(2S) = -66.2(0.3)(19.7) \quad [-80.2(0.3)(33.7)]. \quad (\text{D8})$$

For the logarithmic coefficient B_{61} , we are including previously neglected light-by-light contributions, evaluated in Ref. [78, 79], see Ref. [80]:

$$B_{61}^{\text{LbL}}(nS) = -\frac{43}{36} + \frac{709\pi^2}{3456}. \quad (\text{D9})$$

We checked that using instead of $B_{60}(1S)$ the all-order in $(Z\alpha)$ coefficient [80],³

$$G_{60}(1S) = -94.5(6.6), \quad (\text{D10})$$

the result changes marginally, to -0.520 kHz. This is within the uncertainty estimate in Eq. (D5). For a discussion of the pure SE contribution to G_{60} see Ref. [81].

3. Three-loop SE, electronic VP, and combined effects:

$$\Delta\nu_3 = -0.001 \text{ kHz} \quad [-0.001 \text{ kHz}]. \quad (\text{D11})$$

Including C_{50} and C_{62} from Ref. [82, 83], see Ref. [80]:

$$C_{50}(nS) = -3.3(10.5) \quad [\pm 30], \quad (\text{D12})$$

$$C_{62}(nS) = -\frac{2}{3}B_{40}(nS) \simeq -0.36, \quad (\text{D13})$$

in addition to the leading C_{40} term, has no effect at the precision given above. Note that the four-loop QED contribution has been calculated in Ref. [84], but can be neglected at the present level of precision.

4. Salpeter recoil correction:

$$\Delta\nu_4 = 1032.65 \text{ kHz} \quad [1032.65 \text{ kHz}]. \quad (\text{D14})$$

5. Higher-order pure recoil corrections:

$$\begin{aligned} \Delta\nu_5 &= (-3.140 + 0.081) \text{ kHz} \\ &= -3.059(7) \text{ kHz} \quad [-3.41(32) \text{ kHz}]. \end{aligned} \quad (\text{D15})$$

In Ref. [45], pure recoil corrections at first order in the electron–nucleus mass ratio and expanded up to $(Z\alpha)^7 \log^2(Z\alpha)^{-2}$ in the $(Z\alpha)$ expansion were included. The uncertainty was estimated assuming that the first neglected higher-order term proportional to $(Z\alpha)^7 \log(Z\alpha)^{-2}$ is of natural size. In Ref. [85], it was shown that the previously neglected coefficient D_{71} multiplying the $(Z\alpha)^7 \log(Z\alpha)^{-2}$ term is about a factor 16 larger than the coefficient D_{72} multiplying the supposedly more important $(Z\alpha)^7 \log^2(Z\alpha)^{-2}$ term. This resolved a discrepancy between numerical all-order and analytical $(Z\alpha)$ -expansion results. Here, we use the all-order result reported in Ref. [86]. The two values in Eq. (D15) are the recoil corrections for point-like and Gaussian distributed nuclear charges, respectively. The uncertainty is due to the latter contribution of the nuclear-finite size. As suggested in Ref. [85], we estimate that the uncertainty of the dimensionless parameter $\delta_{\text{fns}}P$ due to the values of the nuclear radii is given by ${}^{2\delta R/R} \delta_{\text{fns}}P$, where for δR we take the difference between the proton and deuteron radii in the Gauss nuclear model and the experimental values from Eqs. (59) and (2). Furthermore, we include an uncertainty due to approximations made in the calculation of $\delta_{\text{fns}}P$ (19×10^{-7} for H, 65×10^{-7} for D) and the difference between the nuclear models in Ref. [85, 86].

6. Radiative recoil corrections:⁴

$$\Delta\nu_6 = -5.38(32) \text{ kHz} \quad [-5.38(11) \text{ kHz}]. \quad (\text{D16})$$

³ This is in agreement with $G_{60}(1S) = -92(13)$ [68].

⁴ Note that the reference for this correction given in Ref. [45] is incorrect. It is calculated from Eq. (56) of Ref. [48].

As suggested in Ref. [87], the more conservative uncertainty estimate from CODATA is used [10].

7. Nuclear SE:

$$\Delta\nu_7 = 2.98(11) \text{ kHz} \quad [2.98(10) \text{ kHz}], \quad (\text{D17})$$

8. Muonic and hadronic VP:

$$\Delta\nu_8 = 0.006 \text{ kHz} \quad [0.006 \text{ kHz}], \quad (\text{D18})$$

While the numerical value of the sum of muonic and hadronic VP contributions remains unchanged, it has in fact been improved, including in addition the effect of NLO hadronic VP and the muonic VP correction to the electromagnetic electron vertex [55]. We checked that the scatter between theoretical predictions and experimental extraction of the hadronic VP contribution to the muon anomalous magnetic moment a_μ , used as input in Ref. [55], agrees with an updated value based on the new experimental result from Fermilab [88] and the presently recommended Standard Model prediction collected in the Theory Initiative White Paper [89]. It also covers the recent lattice QCD prediction from the BMW Collaboration [90]. The further improvement in precision of the scatter is not relevant at the level of precision required for the isotope shift.

9. Nuclear-polarizability correction:

$$\begin{aligned} \Delta\nu_9 &= \left[18.489 - 0.769 I_1^{C0s} \right] \text{ kHz} \\ &= 18.490(205) \text{ kHz} \quad [18.64(2) \text{ kHz}], \end{aligned} \quad (\text{D19})$$

from combining our results in Eqs. (51) and (55). The uncertainty is dominated by $\Delta\nu_9^D$. The decrease of the central value is mainly due to our new \not{x} EFT prediction of the inelastic contribution to the 2γ exchange in D. The error estimate in Ref. [45] seems to be too low by about a factor of 4; based on Eqs. (17) and (18) from Ref. [48], one should get 0.08 kHz instead of 0.02 kHz. In addition, we think that the previously used work [49] might have underestimated the uncertainty. The error estimate presented here is a conservative choice, given the smallness of higher-order terms (in particular, the effect of single-nucleon contributions). We also do not take into account the correlation between the proton contributions in H and D, which would lead to a reduction of the uncertainty estimate.

10. Compensation of the Darwin–Foldy term for the deuteron:

$$\Delta\nu_{10} = 11.37 \text{ kHz} \quad [11.37 \text{ kHz}], \quad (\text{D20})$$

The total contribution to the isotope shift coming from this Set (ii) is given by:

$$\begin{aligned} \Delta f_{ii} &= \left[-4502.48 - 0.769 I_1^{C0s} \right] \text{ kHz} \\ &= -4502.48(40) \text{ kHz} \quad [-4502.66(60) \text{ kHz}], \end{aligned} \quad (\text{D21})$$

where we added the above uncertainties quadratically.

Finally, the smallest correction comes from Set (iii) in Ref. [45]. In the following, we will split the set and separate the contributions that we deduce directly by scaling the leading non-relativistic nuclear-size correction:

$$\Delta f_{iv} = -\frac{7}{24\pi} \frac{\alpha^4 m_e^3 c^4}{\hbar^3} \left[\frac{r_d^2}{(1 + m_e/M_d)^3} - \frac{r_p^2}{(1 + m_e/M_p)^3} \right]. \quad (\text{D22})$$

The higher-order nuclear-size corrections of Set (iii) are:

(b) Elastic contribution to the 2γ exchange:

$$\begin{aligned} \Delta\nu_{(b)} &= \left[0.590 - 1.607 I_1^{C0s} \right] \text{ kHz} \\ &= 0.587(9) \text{ kHz} \quad [0.472 \text{ kHz}], \end{aligned} \quad (\text{D23})$$

from combining our results in Eqs. (52) and (54). The previous result only included the dominant Friar-radius correction.

(c) Relativistic higher-order corrections:

$$\Delta\nu_{(c)} = -2.029(41) \text{ kHz} \quad [-2.828 \text{ kHz}], \quad (\text{D24})$$

Here, we use the recent update from Ref. [87], including the 3γ -exchange effects due to finite nuclear size.

(d) SE contribution to the nuclear size correction:

$$\begin{aligned} \Delta\nu_{(d)} &= \alpha^2 \left[4 \ln 2 - \frac{23}{4} \right] \Delta f_{iv} \\ &= 0.830 \text{ kHz} \quad [0.828 \text{ kHz}]. \end{aligned} \quad (\text{D25})$$

To illustrate the numerical size of the effect, we are using the proton charge radius from the μH Lamb shift, $r_p(\mu\text{H})$ in Eq. (59), and the CODATA 2018 recommended deuteron charge radius, $r_d(\text{CODATA '18})$ in Eq. (3).

(e) Electronic VP contribution to the nuclear size correction:

$$\Delta\nu_{(e)} = \frac{3\alpha^2}{4} \Delta f_{iv} = -0.209 \text{ kHz} \quad [-0.209 \text{ kHz}]. \quad (\text{D26})$$

In total, Set (iii) amounts to:

$$\begin{aligned} \Delta f_{iii} &= \Delta\nu_{(b)} + \Delta\nu_{(c)} + \Delta\nu_{(d)} + \Delta\nu_{(e)} \\ &= -0.821(42) \text{ kHz} \quad [-1.73 \text{ kHz}], \end{aligned} \quad (\text{D27a})$$

Table 9 Individual contributions to the $2S-1S$ transition in H with $R_{\infty c}$ from Eq. (E4)

Contribution	Value (uncertainty) in Hz
Dirac eigenvalue	$\Delta f_1^H = 2\,466\,068\,540\,936\,672$ (2 026)
One-loop SE and electronic VP	$\Delta v_1^H = -7\,124\,094\,961$ (1)
Two-loop SE, electronic VP, and combined effects	$\Delta v_2^H = -636\,881$ (1 733)
Three-loop SE, electronic VP, and combined effects	$\Delta v_3^H = -1\,509$ (370)
Salpeter recoil correction	$\Delta v_4^H = -2\,068\,223$
Higher-order pure recoil corrections	$\Delta v_5^H = 6\,354$ (7)
Radiative recoil corrections	$\Delta v_6^H = 10\,781$ (74)
Nuclear SE	$\Delta v_7^H = -4\,034$ (141)
Muonic and hadronic VP	$\Delta v_8^H = 7\,410$ (70)
Nuclear polarizability correction	$\Delta v_9^H = 41$ (16)
Subtotal: Lamb shift contributions	$\Delta f_{ii}^H = -7\,126\,781\,023$ (1 780)
Elastic 2γ	$\Delta v_{(b)}^H = 35$ (6)
Relativistic higher-order corrections	$\Delta v_{(c)}^H = -928$ (344)
SE contribution to the nuclear size correction	$\Delta v_{(d)}^H = 217.0 \left(\frac{r_p}{\text{fm}}\right)^2$
Electronic VP contribution to the nuclear size correction	$\Delta v_{(e)}^H = -54.7 \left(\frac{r_p}{\text{fm}}\right)^2$
Subtotal: higher-order nuclear-size correction	$\Delta v_{(b)}^H + \Delta v_{(c)}^H = -893$ (344)
	$\Delta v_{(d)}^H + \Delta v_{(e)}^H = 162.3 \left(\frac{r_p}{\text{fm}}\right)^2$
Leading non-relativistic nuclear-size correction	$\Delta f_{iv}^H = -1\,368\,229 \left(\frac{r_p}{\text{fm}}\right)^2$

with

$$\begin{aligned} \Delta v_{(b)} + \Delta v_{(c)} &= \left[-1.439 + 1.607 l_1^{C0s}\right] \text{ kHz} \\ &= -1.442(42) \text{ kHz} \quad [-2.356 \text{ kHz}], \end{aligned} \quad (\text{D27b})$$

$$\begin{aligned} \Delta v_{(d)} + \Delta v_{(e)} &= \alpha^2 [4 \ln 2 - 5] \Delta f_{iv} \\ &= 0.621 \text{ kHz} \quad [0.619 \text{ kHz}]. \end{aligned} \quad (\text{D27c})$$

Here, we again assumed $r_p(\mu\text{H})$ and $r_d(\text{CODATA '18})$ to illustrate the numerical size of the effect.

Collecting Eqs. (D2), (D21), (D27) and (D22), our final result for the theoretical prediction of the $2S-1S$ H-D isotope shift reads:

$$\begin{aligned} f_{\text{iso}} &= \Delta f_i + \Delta f_{ii} + \Delta f_{iii} + \Delta f_{iv} \\ &= \left[671\,000\,534.811(411)(828) + 0.838 l_1^{C0s} \right. \\ &\quad \left. - 1369.346 \left(\frac{r_d}{\text{fm}}\right)^2 \right] \text{ kHz}, \end{aligned} \quad (\text{D28})$$

where the first uncertainty is the combined uncertainty of $\Delta f_i - \Delta f_{iii}$, and the second uncertainty is due to $r_p(\mu\text{H})$ in Δf_{iv} .

Appendix E: Rydberg constant from $2S-1S$ transition in hydrogen and muonic hydrogen Lamb shift

Analogously to Appendix D, we study the S -level transition in H:

$$E_{2S-1S}^H = h f_{2S-1S}^H. \quad (\text{E1})$$

The individual contributions are listed in Table 9. In total, we find:

$$\begin{aligned} f_{2S-1S}^H &= \Delta f_i^H + \Delta f_{ii}^H + \Delta f_{iii}^H + \Delta f_{iv}^H \\ &= \left[0.74960091418756 \frac{R_{\infty c}}{\text{Hz}} - 7\,126\,781\,916(1\,813) \right. \\ &\quad \left. - 1\,368\,229 \left(\frac{r_p}{\text{fm}}\right)^2 \right] \text{ Hz}. \end{aligned} \quad (\text{E2})$$

If not specified differently in Appendix D, we follow the CODATA procedure for the error estimate [10]. For Δf_i , we use the exact formula to deduce the uncertainty, see Ref. [45, Sec. III C.]. We can use Eq. (E2) and $r_p(\mu\text{H})$ to extract the Rydberg constant from the measured transition [91]:

$$f_{2S-1S}^H = 2\,466\,061\,413\,187\,035(10) \text{ Hz}. \quad (\text{E3})$$

Our result:

$$R_{\infty c} = 3.289\,841\,960\,2509(27) \times 10^{15} \text{ Hz}, \quad (\text{E4})$$

is in perfect agreement with Ref. [8, Eq. (22)] and Eq. (D1). Compared to the latter, the uncertainty is more than a factor 2 better. We can use this value to extract the deuteron radius from the $2S-1S$ transition in D, since it is largely driven by the measured Lamb shift in μH .

Table 10 Individual contributions to the $2S-1S$ transition in D with $R_{\infty}c$ from Eq. (E4)

Contribution	Value (uncertainty) in Hz
Dirac eigenvalue	$\Delta f_1^D = 2\,466\,739\,545\,007\,700$ (2 025)
One-loop SE and electronic VP	$\Delta v_1^D = -7\,129\,653\,960$ (1)
Two-loop SE, electronic VP, and combined effects	$\Delta v_2^D = -637\,402$ (1 734)
Three-loop SE, electronic VP, and combined effects	$\Delta v_3^D = -1\,510$ (370)
Salpeter recoil correction	$\Delta v_4^D = -1\,035\,575$
Higher-order pure recoil corrections	$\Delta v_5^D = 3\,295$ (3)
Radiative recoil corrections	$\Delta v_6^D = 5\,398$ (37)
Nuclear SE	$\Delta v_7^D = -1\,059$ (35)
Muonic and hadronic VP	$\Delta v_8^D = 7\,416$ (70)
Nuclear polarizability correction	$\Delta v_9^D = 18\,531$ (204)
Compensation of the Darwin–Foldy term for the deuteron	$\Delta v_{10}^D = 11\,369$
Subtotal: Lamb shift contributions	$\Delta f_{ii}^D = -7\,131\,283\,498$ (1 787)
Elastic 2γ	$\Delta v_{(b)}^D = 622$ (7)
Relativistic higher-order corrections	$\Delta v_{(c)}^D = -2\,961$ (357)
SE contribution to the nuclear size correction	$\Delta v_{(d)}^D = 217.1 \left(\frac{r_d}{\text{fm}}\right)^2$
Electronic VP contribution to the nuclear size correction	$\Delta v_{(e)}^D = -54.7 \left(\frac{r_d}{\text{fm}}\right)^2$
Subtotal: higher-order nuclear-size correction	$\Delta v_{(b)}^D + \Delta v_{(c)}^D = -2\,340$ (357)
	$\Delta v_{(d)}^D + \Delta v_{(e)}^D = 162.4 \left(\frac{r_d}{\text{fm}}\right)^2$
Leading non-relativistic nuclear-size correction	$\Delta f_{iv}^D = -1\,369\,346 \left(\frac{r_d}{\text{fm}}\right)^2$

Appendix F: $2S-1S$ transition in deuterium

Analogously to Appendix E, we study the S -level transition in D:

$$E_{2S-1S}^D = h f_{2S-1S}^D \tag{F1}$$

The individual contributions are listed in Table 10. For the 3γ -exchange contribution, we use Ref. [87, Eq. (104)] with $r_d(\mu\text{D})$ from Eq. (4) and apply 10% uncertainty for the inelastic part and 100% for the single-nucleon part, where for the latter we also assume a correlation between $1S$ and $2S$ levels. The updated theory prediction for the $2S-1S$ transition in D, including the 2γ exchange from $\not\{EFT}$, then reads:

$$f_{2S-1S}^D = \Delta f_i^D + \Delta f_{ii}^D + \Delta f_{iii}^D + \Delta f_{iv}^D = \left[2\,466\,732\,413\,721\,862(2\,724) - 1\,369\,346 \left(\frac{r_d}{\text{fm}}\right)^2 \right] \text{Hz} \tag{F2}$$

This is used in Sect. 6.1 to extract the deuteron charge radius.

Appendix G: Neutron charge radius and deuteron structure radius

Another interesting quantity is the deuteron structure radius, defined as:

$$r_{\text{str}}^2 = r_d^2 - 2r_0^2 \tag{G1}$$

This definition implies that the difference of squared deuteron and proton charge radii is related to the sum of squared deuteron structure radius and neutron charge radius:

$$r_d^2 - r_p^2 = r_{\text{str}}^2 + \frac{3}{4M_p^2} + r_n^2 \tag{G2}$$

The deuteron structure radius has recently been predicted in χET [27]:

$$r_{\text{str}}(\chi\text{ET}) = 1.9729 \left(\begin{smallmatrix} +15 \\ -12 \end{smallmatrix} \right) \text{fm} \tag{G3}$$

We can use this value as an alternative reference to fix the unknown LEC from Eq. (15):

$$l_1^{C0s} = -2.41 \left(\begin{smallmatrix} +32 \\ -26 \end{smallmatrix} \right) (35) \times 10^{-3} = -2.41 \left(\begin{smallmatrix} +48 \\ -44 \end{smallmatrix} \right) \times 10^{-3}, \tag{G4}$$

where the first error is due to r_{str} and the second is due to Z . Using in addition the $2S-1S$ H–D isotope shift in Eq. (D28), we extract the neutron charge radius as:

$$r_n^2 = -0.105 \left(\begin{smallmatrix} +5 \\ -6 \end{smallmatrix} \right) \text{fm}^2, \tag{G5}$$

in exact agreement with Ref. [27], but in slight disagreement with the value used by us, see Eq. (31). We checked that the effect of the nucleon charge radii entering our $\not\{EFT}$ prediction of the 2γ exchange adds up to 0.021 kHz. Since the size of these nucleon-radius contributions is covered by the

uncertainty budget in Eq. (58), we can safely ignore this correlation in the above extraction of r_n . Note that even though the value of l_1^{C0s} in Eq. (G3) agrees well with Eq. (16), the corresponding values for r_d disagree, since it also depends on r_n through r_0 , cf. Eq. (15).

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