Theory of the $n = 2$ levels in muonic deuterium

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The present knowledge of Lamb shift, fine- and hyperfine structure of the 2S and 2P states in muonic deuterium is reviewed in anticipation of the results of a first measurement of several 2S − 2P transition frequencies in muonic deuterium ($\mu d$). A term-by-term comparison of all available sources reveals reliable values and uncertainties of the QED and nuclear structure-dependent contributions to the Lamb shift, which are essential for a determination of the deuteron rms charge radius from $\mu d$. Apparent discrepancies between different sources are resolved, in particular for the difficult two-photon exchange contributions. Problematic single-sourced terms are identified which require independent recalculation.

I. INTRODUCTION

Laser spectroscopy of $2S \rightarrow 2P$ Lamb shift transitions in muonic atoms and ions promises a tenfold improvement in our knowledge of charge and magnetic radii of the lightest nuclei ($Z = 1, 2$ and higher). Our recent measurement [1, 2] of the 2S Lamb shift and the 2S hyperfine splitting (HFS) in muonic hydrogen, $\mu p$, in combination with accurate theoretical calculations by many authors, summarized in Ref. [3], has revealed a proton root-mean-square (rms) charge radius of

$$r_p = 0.84087 \ (26)_{\text{exp}} \ (29)_{\text{theo}} \text{ fm} = 0.84087 \ (39) \text{ fm}. \quad (1)$$

This is an order of magnitude more accurate than the value of $r_p = 0.8775(51) \text{ fm}$ evaluated in the CODATA least-squares adjustment [4] of elastic electron-proton scattering [5, 6] and many precision measurements in electronic hydrogen [7].

Most strikingly, however, the two values differ by 7 combined standard deviations (7σ). Despite numerous attempts in recent years to explain this “proton radius puzzle”, it remains a mystery [8, 9]. Taken at face value, this 7σ discrepancy constitutes one of the biggest discrepancies in the Standard Model. Further data are clearly required to shed light on this puzzle.

Muonic deuterium, $\mu d$, has been measured in the same beam time as $\mu p$ [1, 2], and the data are now nearing publication [10]. We anticipate here that the experimental accuracy of the various 2S − 2P transitions is of the order of 1 GHz, or, equivalently, $\sim 0.004 \text{ meV}$ [1]. Ideally, theory should be accurate on the level of 0.001 meV to exploit the experimental precision, and to determine the deuteron charge radius, $r_d$, with tenfold better accuracy, compared to the CODATA value [4]

$$r_d \ (\text{CODATA}) = 2.1424(21) \text{ fm}. \quad (2)$$

The CODATA value originates from a least-squares adjustment of a huge amount of input values, such as the proton radius from electron scattering [5, 6]. These radii are connected because the CODATA adjustment includes many transition frequencies in hydrogen (H) and deuterium (D) [4, 7]. In particular, the squared deuteron-proton charge radius difference,

$$r_d^2 - r_p^2 = 3.82007 \ (65) \text{ fm}^2 \quad (4)$$

is known with high precision from laser spectroscopy of the isotope shift of the $1S − 2S$ transition in electronic hydrogen and deuterium [13], and state-of-the-art theory [14]. Using Eq. (4) and the muonic hydrogen proton radius given in Eq. (1) we determined a value of [2]

$$r_d \ (\text{muonic } r_p) = 2.12771 \ (22) \text{ fm}. \quad (5)$$

Note that the discrepancy of the deuteron charge radii given in Eq. (2) and Eq. (5) is not a new discrepancy,
but rather a result of the proton radius discrepancy: Both values of the deuteron radius depend on the isotope shift in Eq. (4). Hence, discrepant values of the proton radius will result in discrepant values of the deuteron radius.

The upcoming $\mu d$ data \cite{10}, on the other hand, will provide a “muonic” value of the deuteron radius that is independent of the proton charge radius. As such, it will shed new light on the proton radius puzzle.

We anticipate here that the theory of the Lamb shift in muonic deuterium is limiting the accuracy of the deuteron charge radius from $\mu d$, mainly due to the uncertainty of the deuteron polarizability contribution of 0.020 meV which corresponds to a relative uncertainty of 1%. Nevertheless, the deuteron charge radius from $\mu d$ \cite{10} will have a nearly three times smaller uncertainty than the current CODATA value (Eq. (2)).

To put this uncertainty of 0.020 meV into another perspective: The “proton radius puzzle” in muonic hydrogen, when expressed as a “missing part” in the theory of muonic hydrogen, amounts to 0.329 meV.

This article is organized as follows: We first summarize the current knowledge of the muonic deuterium Lamb shift theory (Sec. III) which is required to determine the deuteron rms charge radius $r_d$ from the $\mu d$ measurement \cite{10}. We separate the Lamb shift theory into “radius-independent” terms that do not depend on the nuclear structure (Sec. IIIA), terms that depend explicitly on the rms charge radius (Sec. IIIB), and the deuteron polarizability contribution that constitutes the main theoretical limitation (Sec. IIIC). In Sec. IV we list all contributions to the 2S hyperfine splitting (HFS) in $\mu d$. The 2S HFS depends on the magnetic properties of the deuteron through the Zemach radius. Other nuclear structure contributions matter, too, so we separate again terms: Sec. IVB lists the terms that do not depend strongly on the deuteron structure, Sec. IVC is devoted to the Zemach correction, Sec. IVD is concerned with the deuteron polarizability contribution which has recently been calculated for the first time \cite{19}. This term constitutes the main uncertainty for the 2S HFS prediction. Additional contributions to the 2S HFS are mentioned in Sec. IVF. The 2P fine structure is summarized in Sec. V and the 2P fine- and hyperfine level structure, including level mixing, is given in Sec. VI.

The sign convention in this article is such that the final, measured energy difference (Lamb shift, 2S-HFS, fine structure) is always positive. For the fine and hyperfine splittings this convention is the natural choice adopted by all other authors, too. For the Lamb shift, however, some authors calculate 2S level shifts and their published values have the opposite sign. This is because the 2S level is lower (more bound) than the 2P level (due to the dominant vacuum-polarization term item #1 in Tab. I), see Fig. I and positive level shifts decrease the measured 2P-2S energy difference. The numbers we quote are all matched to our sign convention.

Item numbers # in the first column of Tab. I and Tab. V follow the nomenclature in Ref. \cite{3}. In the tables, we usually identify the “source” of all values entering “our choice” by the first name of the (group of) authors given in adjacent columns (e.g. “B” for Borie). We denote as average “avg.” in the tables the center of the band covered by all values $v_i$ under consideration, with an uncertainty of half the spread, i.e.

$$\text{avg.} = \frac{1}{2} \left[ \text{MAX}(v_i) + \text{MIN}(v_i) \right]$$

$$\pm \frac{1}{2} \left[ \text{MAX}(v_i) - \text{MIN}(v_i) \right]$$

Throughout the paper, $Z$ denotes the nuclear charge with $Z = 1$ for the deuteron, $\alpha$ is the fine structure constant, $m_\mu$ is the reduced mass of the muon-deuteron system. “VP” is short for “vacuum polarization”, “SE” is “self-energy”, “RC” is “recoil correction”. “Perturbation theory” is abbreviated as “PT”, and SOPT and TOPT denote 2nd and 3rd order PT, respectively.

II. OVERVIEW

The $n = 2$ levels in muonic deuterium are sketched in Fig. I. The Lamb shift, i.e. the splitting between the 2S and the 2P$_{1/2}$ state, is sensitive to the rms charge radius of the deuteron, as detailed in Sec. III. In contrast, 2S hyperfine splitting (HFS) is caused by the magnetic interaction between the muon spin and the magnetic moment of the deuteron. The finite deuteron size results in a finite magnetization distribution inside the deuteron, and makes the 2S HFS depend on the so-called Zemach radius of the deuteron, as explained in Sec. IV.

The first calculation of the Lamb shift in muonic deuterium was published by Carboni \cite{16} in 1973. More elaborate calculations of QED effects in muonic atoms were introduced with the seminal paper by Borie and Rinker \cite{17} in 1982.

Later, Pachucki \cite{18} and Borie \cite{19} presented very detailed calculations of many terms for muonic hydrogen. Borie then extended her $\mu p$ calculations \cite{19} to the case...
of muonic deuterium \[20\]. After our measurements in muonic hydrogen \[12\] and deuterium, Borie revisited the theory of the \(n = 2\) energy levels in light muonic atoms (\(\mu p, \mu d, \mu^3\text{He},\) and \(\mu^4\text{He}\)) in Ref. \[21\]. The published paper \[21\] (available online 6 Dec. 2011) has subsequently been superseded by the arXiv version of the paper \[22\]. At the time of this writing, Borie’s paper on the arXiv has reached version 7 (dated 21 Aug. 2014). This is the first source of knowledge on \(\mu d\) summarized in here.

The second source is the group around Faustov, Kru-tov, Martynenko et al., termed “Martynenko” in here for simplicity. They have published an impressive set of papers on theory of energy levels in light muonic atoms. At the time of this writing, the 2011 paper \[23\] was the most recent one on the Lamb shift in \(\mu d\), and we based our summary on this paper. Later, Ref. \[24\] from the Martynenko group appeared, with only minor differences in the results compared to Ref. \[23\]. For simplicity, we still base our compilation of Lamb shift contributions on the earlier, more detailed, paper \[23\]. In particular, equation numbers and table entries refer to Ref. \[23\], unless otherwise noted. For the 2S HFS, Ref. \[15\] is the main source of numbers from the Martynenko group.

After the advent of the proton radius puzzle from muonic hydrogen, many groups have revisited and improved the theory on muonic hydrogen in an (unsuccessful) attempt to identify wrong or missing theory terms large enough to solve the puzzle (see our compilation \[3\] for a detailed overview). Thankfully, two groups have (re-)calculated many terms not only for the case of muonic hydrogen, but also for muonic deuterium (and \(\mu^3\text{He}\) and \(\mu^4\text{He}\)): Jentschura, and Karshenboim’s group with Ivanov, Korzinin, and Shelyuto, have published many papers on muonic deuterium which are included in the present compilation.

III. LAMB SHIFT IN MUONIC DEUTERIUM

A. QED contributions

One-loop electron vacuum polarization (eVP) (Fig. 2), the so-called Uehling term \[25\], accounts for 99.5 % of the nuclear-structure-independent part of the Lamb shift in \(\mu d\). It is therefore mandatory to double-check this term as thoroughly as possible.

Borie has argued \[17, 20–22\] that the Uehling term should ideally not be treated perturbatively. Instead, the Dirac equation should be solved numerically after adding the Uehling potential to the electrostatic Coulomb potential. For light muonic atoms such as muonic deu-
FIG. 2. Item #1, the leading order 1-loop electron vacuum polarization (eVP), also called Uehling term.

terium, however, both approaches should give accurate results [22]. This has been demonstrated for muonic hydrogen, where the nonperturbative result of Indelicato [26] is in excellent agreement with the perturbative results of Pachucki [18] and Borie [19], see Ref. [3].

For muonic deuterium, only perturbative calculations exist, albeit with two slightly different approaches:

Martynenko et al. [23], Jentschura [27, 28] and Karshenboim et al. [29, 30] calculate the leading order eVP nonrelativistically (item #1 in Tab. I), and apply a relativistic correction (item #2). The most important item #1 is in excellent agreement for all three authors, as well as with the value of 227.635 meV obtained by Carboni [16] in 1973. For item #2 see below.

Borie, in contrast, uses relativistic Dirac wave functions to evaluate the relativistic Uehling term (item #3). The relativistic recoil correction to eVP of order $\alpha(Z\alpha)^4$ (item #19) has to be added, to be able to compare all four results.

It is very reassuring that these results are in excellent agreement, with one exception: Item #2, rel. corr. (Breit-Pauli), from Martynenko [23], 0.0177 meV, differs from the value of 0.02178 meV, calculated by the other three groups, who agree: Borie [22] Tab. 1, Jentschura [31] Tab. I and [28] Eq. (17), and Karshenboim [30] Tab. IV. Martynenko confirmed that their value for our item #2 for muonic deuterium (their rows 7 and 10 in Tab. I of Ref. [23]) contains an error [33]. The average of items #1+#2 or #3+#19 is thus calculated from the other three sources only, with excellent agreement:

$$\Delta E \text{ (one \textit{--} loop eVP with rel. corr.)} = 227.65658 \pm 0.00020 \text{ meV} \quad (7)$$

Our item #4, the two-loop electron-VP correction, usually called “Källen-Sabry” contribution [34], displayed in Fig. 3 is the second largest “purely QED” contribution to the Lamb shift. Borie [22] and Martynenko [23] give values which are in very good agreement.

Our item #5, the one-loop eVP insertion in 2 Coulomb lines shown in Fig. 4 has been calculated with very good agreement by Borie [22], Martynenko [23], and Jentschura [28].

Karshenboim et al. [29] give the sum of items #4 and #5. It is in agreement with the sums from Borie and Martynenko. We use Karshenboim’s value because it is given with more significant digits.

FIG. 3. Item #4, the two-loop eVP (Källen-Sabry) contribution.

FIG. 4. Item #5, the one-loop eVP in 2-Coulomb lines.

VP corrections of order $\alpha(Z\alpha)^2$ in first and second order PT). For muonic helium-3 and -4 ions [32] the sum agrees exactly with the numbers given by Jentschura in Ref. [27] Eq. (17) and by Karshenboim in Ref. [30] Tab. IV. Martynenko confirmed that their value for our item #2 for muonic deuterium (their rows 7 and 10 in Tab. I of Ref. [23]) contains an error [33]. The average of items #1+#2 or #3+#19 is thus calculated from the other three sources only, with excellent agreement:

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FIG. 5. The three contributions to Light-by-light scattering: (a) Wichmann-Kroll or “1:3” term, item #9, (b) Virtual Delbrück or “2:2” term, item #10, and (c) inverted Wichmann-Kroll or “3:1” term, item #9a. 
Light-by-light (LbL) scattering (see Fig. 5) contains 3 terms, Wichmann-Kroll, or “1:3” LbL (item #9 in \[3\]), Virtual Delbrück, or “2:2” LbL (item #10 in \[3\]), and the “inverted Wichmann-Kroll” or “3:1” LbL (called “new” item in \[3\]). For definiteness, we label this term “item #9a” from now on. Considerable cancellations occur in the sum of all three terms which has been evaluated in Ref. \[35\]. Both Borie and Martynenko calculate only #9, and adopt the full result from Karshenboim \[35\]. We use Karshenboim’s result \[35\].

Item #11 muon self-energy (SE) correction to electron vacuum polarization \(\alpha^2(Z\alpha)^4\) is displayed in Fig. 6. Jentschura \[28\] (Eq. (29b), Fig. 2) and Karshenboim \[37\] (Tab.VIII (a), Fig. 6a) agree in the result for the complete calculation, -0.00306 meV. Martyonenko \[23\] Eq. (80) calculates only the contribution from Fig. 6(a), following Pachucki’s Eq. (39) in Ref. \[18\]. Also Borie \[22\] calculates part of this term in her Appendix C.

Higher order corrections to the muon self-energy and vacuum polarization are denoted items #12, #13, #21, #30\(^*\) and #31\(^*\) in Tab. I. For muonic hydrogen \[3\] we used Borie’s value of item #21, noting that this includes item #12. Afterwards, Karshenboim \[37\] have recalculated many of these small terms. We construct the corresponding sum from each source, which we average. Item #12 is shown in Fig. 7. It is Martynenko’s item 29. This contribution has been confirmed by Karshenboim \[37\] Tab. VIII (d). As mentioned in Ref. \[3\], item #12 is included in Borie’s value for item #21.

Item #13, mixed muon-electron VP is depicted in Fig. 8. Borie and Martynenko calculated only the contribution from Fig. 8(a), see Fig. 3 in Ref. \[38\]. This is Martynenko’s item 3, “VP and MVP contribution in one-photon interaction”. Karshenboim gives the sum of both diagrams in Fig. 8 in Ref. \[37\] Tab. VIII (d).

Item #30\(^*\) (#31\(^*\)) is somewhat similar to item #12 (#13), with the electron (muon) loop replaced by a hadronic VP loop, see Fig. 9. It has only been calculated by Karshenboim \[37\], Tab. VIII item (e) ((c)). Item #32, the muon VP in SE correction shown in Fig. 11 is not included as a separate item in our Tab. \[1\] It should already be automatically included in any QED value which has been rescaled from the QED of electronic deuterium by a simple mass replacement \(m_e \rightarrow m_\mu\) \[39\]. The size of this item #32 can be estimated from the relationship found by Borie \[40\], that the ratio of hadronic to muonic VP is 0.66. With Karshenboim’s value of item #30\(^*\) \[37\] one would get \(\Delta E(#32) = -0.000024/0.66\) meV = -0.000036 meV.

Item #21, higher order correction to \(\mu SE\) and \(\mu VP\), is Borie’s muon Lamb shift, higher orders, calculated in her Appendix C of Ref. \[22\]. This item includes item #12, \(eVP\) loop in \(\mu SE\) correction of \(\alpha^2(Z\alpha)^4\), as explained on p. 131 of Ref. \[3\].

The sum of items #12, #13, #21, #30\(^*\) and #31\(^*\) agree well enough to justify taking the average, \(-0.00178 \pm 0.00014\) meV as our choice.

Item #14, hadronic VP, is evaluated by Borie \[22\] (p. 5) as 0.013 meV, who assigns a 5% uncertainty to this estimate which is based on Refs. \[17, 40–42\]. Martyonenko’s value of 0.0129 meV \[23\], Tab. 1, row 31, agrees very nicely. They quote Ref. \[41, 43\], and estimate the uncertainty to 5% as well.

The previous items #15 and #16 in Ref. \[3\] are higher order corrections to the hadronic VP and have only been calculated for muonic hydrogen by Martyonenko’s

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2 There is a typo in footnote f of Tab. 1 in Ref. \[3\], where we wrote, item #12 “is part of #22” (instead of #21).

3 The asterisk * indicates that this item had not been considered for muonic hydrogen in Ref. \[3\].
FIG. 8. Item #13, the mixed eVP-$\mu$VP contribution.

group [44, 45], where they are small (0.000047 meV and -0.000015 meV, respectively). It is expected that their magnitude will be similar in muonic deuterium. Hence these terms are included in the 5% uncertainty assigned to item #14.

Item #18 in Ref. [3] is the recoil finite size contribution in Borie [21, 22]. According to Pachucki, this item #18, which was first calculated by Friar [46], should be discarded [47], as we did for muonic hydrogen in Ref. [3].

Item #17 is the Barker-Glover correction [48], termed additional recoil by Borie. This item includes the Darwin-Foldy (DF) term that arises from the Zitterbewegung of the nucleus. For a spin-1 nucleus such as the deuteron (as well as for the spin-0 $^4$He nucleus) this DF term is absent [49]. Different conventions are used in the literature [50–52] which has caused some confusion (see Appendix A). As in the case of muonic hydrogen [3] (where the DF term is nonzero), we follow the “atomic physics” convention [52], also adopted by CODATA-2010 [4]. In this way, the charge radii from muonic hydrogen [1, 2] and deuterium [10] are directly comparable to the CODATA-2010 values [4], as well as the electronic H-D-isotope shift given in Eq. (4), all of which follow the same convention [13, 14].

Item #28 is the rad. (only eVP) RC $\alpha(Z\alpha)^5$ labeled “new” in Ref. [3]. For definiteness, we enumerate it as item #28'. It is the sum of three individual parts which sum up to 0.000093 meV in Ref. [28], Eq. (46b), Martynenko’s row 26 of Tab. I in Ref. [24], recoil corr.

to VP of order $\alpha(Z\alpha)^3$ (seagull term) is only the seagull term from the three terms evaluated by Jentschura, taken from Ref. [27], Eq. (29). We take the full result from Ref. [28], Eq. (46b).

Item #24 are radiative recoil corrections of order $\alpha(Z\alpha)^5$ and $(Z^2\alpha)(Z\alpha)^4$, first introduced for $\mu p$ by Pachucki [18], Eq. (51), based on Ref. [53]. Borie writes (p. 9 of Ref. [22]) that these terms correspond to Tab. 8 and two additional terms from Tab. 8 of the review of Eides et al. [42]. The sum is -0.00302 meV for $\mu d$. Martynenko et al. (Ref. [23], row 27 of Tab. 1, and Eq. (71)), on the other hand, evaluate only the terms from Tab. 9 of Eides [42], which gives -0.0026 meV. We use Borie’s complete result.

Item #29*, the $\alpha^2(Z\alpha)^4 m$ contribution to the Lamb shift, is new and has not been considered for muonic hydrogen in Ref. [3]. We keep enumerating the items, making this item #29* 3.

Martynenko gives this as the sum of rows 8 and 11 in Tab. 1 of [23], relativistic and two-loop VP corrections of order $\alpha^2(Z\alpha)^4$ in 1st and 2nd order PT. They sum up to $-0.0002 + 0.0004 = 0.0002$ meV. Karshenboim calculated the complete correction of this order, with recoil corrections included and calls it eVP2 in Tab. VIII of Ref. [37]. Their value of 0.000203 meV replaces Martynenko’s rows 8 and 11 [39].

FIG. 9. Item #30*, hadronic VP in SE contribution, corresponds to Fig. 6(e) in Karshenboim [37].

FIG. 10. Item #31*, the mixed eVP- and hadronic VP contribution, comes from the Uehling correction to the hadronic VP correction. See Fig. 6(c) in Karshenboim [37].

FIG. 11. Item #32, muon VP in SE contribution, is automatically included in a rescaled electronic deuterium QED value of higher order SE contributions (see text).
Numerically this item #29 is of little practical importance, because it is so tiny: 0.000173 meV in \( \mu p \), and 0.000203 meV in \( \mu d \). Of course, the calculation of this term was an important confirmation that previously uncalculated higher order terms are not responsible for the proton radius discrepancy. It is very reassuring that the two different approaches of Martynenko \[23\] and Karshenboim \[37\] give the same result. Interestingly, there is no such an agreement for the cases of muonic helium-3 and -4 ions. In view of our recent measurements in muonic helium-3 and -4 \[54\], this disagreement may deserve further study, even though the size of the terms is small compared to the overall uncertainty.

The sum of all contributions without explicit nuclear structure dependence summarized in Tab. \[I\] amounts to

\[
\Delta E_{\text{rad.-indep.}}^{\text{LS}} = 228.77356 \pm 0.00075 \text{ meV.} \quad (8)
\]
TABLE I. All known radius-independent contributions to the Lamb shift in $\mu d$. Values are in meV. Item numbers "#" in the 1st column follow the nomenclature of Ref. [3], which in turn followed the Supplement of Ref. [1]. Items "#" with a dagger $^\dagger$ were labeled "New" in Ref. [3], but we introduce numbers here for definiteness. Items # with an asterisk * denote new contributions in this compilation.

For Borie [22] we refer to the most recent arXiv version-7 (dated 21 Aug. 2014) which contains several corrections to the published paper [21] (available online 6 Dec. 2011). For Martynenko, numbers #1 to #31 refer to rows in Tab. I of Ref. [23]. The values in their more recent paper [24] agree exactly with the earlier values [23]. Numbers in parentheses refer to equations in the respective paper.

| #  | Contribution                                                                 | Borie | Martynenko | Jentschura | Karshenboim | Our choice value source | Fig. |
|----|-----------------------------------------------------------------------------|-------|------------|------------|-------------|------------------------|------|
| 1  | NR one-loop electron VP (eVP)                                              | 227.6347 | #1         | 227.6346   | 227.63467   | 227.65658 ± 0.00020 avg. | 2   |
| 2  | Rel. corr. (Breit-Pauli)                                                  | 0.02178 | Tab. 1     | 0.021781   | 0.021781    | 0.021781               | 29  |
| 3  | Rel. one-loop eVP                                                         | 227.6557 | p. 3 Tab.  | 227.6546   | 227.65545   |                         |     |
| 19 | Rel. RC to eVP, $\alpha(Z\alpha)^4$                                      | -0.00093 | Tab. 1+4   | 227.6568   | 227.6564    |                         |     |
|    | Sum of the above                                                          | (227.6524) |           | 1.8380     | 1.8380      | 1.83804                | Tab. I | 1.83804 | K       |
| 4  | Two-loop eVP (Källén-Sabry)                                               | 1.66622 | p. 3 Tab.  | 1.6660     | #2          | #2                    | 3   |
| 5  | One-loop eVP in 2-Coulomb lines $\alpha^2(Z\alpha)^5$                     | 0.1718  | p. 3       | 0.172023   | 25(13)      | 0.000842(7)            | 29  |
|    | Sum of #4 and #5                                                          | 1.8380  |             | 1.8380     | 1.8380      | 1.83804                | Tab. I | 1.83804 | K       |
| 6+7 | Third order VP                                                            | 0.00842 |           | 0.0086     | #4+12+13    | 0.00842(7)             | 29  |
| 29 | Second-order eVP contribution $\alpha^2(Z\alpha)^4$m                      | 0.0002  | #8+11      | 0.000203   | 0.00020     | 0.00020                | K   |
| 9  | Light-by-light “1:3”': Wichmann-Kroll                                      | -0.00111 | p. 4       | -0.0011    | #5          | -0.001098(4)           | 35  |
| 10 | Virtual Delbrück, “2:2” LbL                                                | 0.0001  | #6         | 0.00124(1) | 0.00124(1)  | 0.00101(10)            | 35  |
| 9a | "3:1" LbL                                                                 | 0.00096 |           | -0.00100   | -0.00096(2) | -0.00096 ± 0.00002 K   |     |
| 20 | $\mu$SE and eVP                                                           | -0.774616 | p. 11 Tab. 2 | -0.7747    | #28         | -0.00306               | 29  |
|    | (−0.00589)                                                               | Tab. 16 |           | -0.0041    | #30         | 25(29)                 |      |
|    | Sum of #12, 13, 31, and 21                                                 | -0.00192 |           | -0.0017    | -0.00164(1) | -0.00178 ± 0.00014 avg. | 6   |
| 14 | Hadronic VP                                                               | 0.013±5 % | p. 5+Tab.4 | 0.0129±5 % | #31         | 0.01290 ± 0.00070 M+B  |     |
| 17 | Recoil corr. : $(Z\alpha)^4)m^2/M^2$(Barker-Glover)                        | 0.06724 | p. 9/10  | 0.06722    | 25(13)      | 0.06723 ± 0.00001 avg. |     |
| 22 | Rel. RC $(Z\alpha)^5$                                                     | -0.02656 | p. 9     | -0.0266    | #24         | -0.02656               | avg  |
| 23 | Rel. RC $(Z\alpha)^6$                                                     | 0.0001  | #25       | 0.0001     | #25         | 0.00010                | M    |
| 24 | Higher order radioactive recoil corr.                                      | -0.00302 | p. 9     | -0.0026    | #27         | -0.00302               | B    |
| 28 | Rad. (only eVP) RC $(Z\alpha)^5$                                          | 0.0002  | #26       | 0.000093   | 25(46)      | 0.000093               | J    |

Sum: 228.7797 ± 0.04 B 228.768 ± 0.00075

a Does not contribute to the sum in Borie’s approach, see text.
b Contains a mistake [33], see text.
c In Appendix C, incomplete.
d Martynenko calculates only a part of this item.
e This item is part of #21 (and not of #22 as we erroneously wrote in Tab. 1, footnote f of Ref. [3]).
f This is only Tab. 9 from Ref. [22], whereas parts of Tab. 8 should be included here, too [22].
g This is only the seagull term [23, 27, 28].

# Contribution
1. NR one-loop electron VP (eVP)
2. Rel. corr. (Breit-Pauli)
3. Rel. one-loop eVP
19. Rel. RC to eVP, $\alpha(Z\alpha)^4$
   Sum of the above
4. Two-loop eVP (Källén-Sabry)
5. One-loop eVP in 2-Coulomb lines $\alpha^2(Z\alpha)^5$
   Sum of #4 and #5
6+7. Third order VP
29. Second-order eVP contribution $\alpha^2(Z\alpha)^4$m
9. Light-by-light “1:3”': Wichmann-Kroll
10. Virtual Delbrück, “2:2” LbL
9a. “3:1” LbL
   Sum: Total light-by-light scatt.
20. $\mu$SE and eVP
11. Muon SE corr. to eVP $\alpha^2(Z\alpha)^4$
12. eVP loop in self-energy $\alpha^2(Z\alpha)^4$
30. Hadronic V loop in self-energy $\alpha^2(Z\alpha)^4$m
13. Mixed eVP + $\mu$VP
31. Mixed eVP + hadronic VP
21. Higher-order corr. to $\mu$SE and eVP
   Sum of #12, 13, 31, and 21
14. Hadronic VP
17. Recoil corr. : $(Z\alpha)^4)m^2/M^2$(Barker-Glover)
22. Rel. RC $(Z\alpha)^5$
23. Rel. RC $(Z\alpha)^6$
24. Higher order radioactive recoil corr.
28. Rad. (only eVP) RC $(Z\alpha)^5$
B. Radius-dependent contributions to the Lamb shift

The radius-dependent contributions to the Lamb shift [22, 24, 30] are listed in Tab. III. Generally, the finite size of the nucleus affects mainly the S states whose wave function is nonzero at the origin, where the nucleus resides. The main finite size contributions to the nS states have been given to order \((Z\alpha)^6\) by Friar [46].

\[
\Delta E_{\text{fin, size}} = \frac{2\pi Z\alpha}{3} |\Psi(0)|^2 \left[ \langle r^2 \rangle - \frac{Z\alpha m_r}{2} \langle r^3 \rangle_{(2)} + \frac{(Z\alpha)^2}{2} (F_{\text{REL}} + m_r^2 F_{\text{NREL}}) \right].
\]  

(9)

Here, \(|\Psi(0)|^2\) denotes the muon wave function at the origin, \(\langle r^2 \rangle\) is the rms charge radius of the nucleus, and \(\langle r^3 \rangle_{(2)}\) is its “Friar moment” [46]. As detailed in Sec. III C there is no contribution from the Friar moment due to a cancelation with part of the inelastic deuteron “polarizability” contributions.

In Eq. (9), \(F_{\text{REL}}\) and \(F_{\text{NREL}}\) contain various moments of the nuclear charge distribution, see Ref. [10], and in particular the Appendix E therein for analytic expressions for some simple model charge distributions.

The leading order finite size effect, item (r1) in Tab. III, is the first term in Eq. (9). It originates from the one-photon exchange with a deuteron form factor insertion shown in Fig. 12 and is proportional to the rms charge radius of the deuteron, \(\langle r_d^2 \rangle\).

![FIG. 12. Item (r1), the leading nuclear finite size correction stems from a one-photon interaction with a deuteron form factor insertion, indicated by the thick dot.](image)

For (r2), the radiative correction \(\alpha(Z\alpha)^5\), we chose Martynenko’s value: The equations for the calculation of this term are given in [57]. Borie [22], Tab. 14 uses Eq. (10) of Ref. [57], which gives the total radiative correction of order \(\alpha(Z\alpha)^5\), i.e. the sum of Eqs. (7) and (9) in Ref. [57]. Martynenko [23], in contrast, uses Eq. (9) of Ref. [57], stating that the additional polarization correction, Eq. (7) in Ref. [57], which is included in Eq. (10), cancels with a part of the (inelastic) deuteron polarizability contribution.

The finite size correction to the Lamb shift of order \((Z\alpha)^6\) has first been calculated by Friar [46], see in particular Appendix E therein. Both Borie [22] (p. 30) and Martynenko [24] (Eq. (33)) follow Friar [46] and evaluate this contribution as the sum of two terms which we list separately:

The first one, (r3), has an explicit \(\langle r_d^2 \rangle\) dependence, while the second one, (r3’), is usually evaluated for an exponential charge distribution, since a model-independent evaluation of this term is prohibitively difficult [22]. Small differences between the formulas given by Borie [22] and Martynenko [24] result in values for (r3’) of 0.0029 meV and 0.0031 meV. For example, the term \(\langle r^2 \rangle \langle \ln(\mu r) \rangle\), which is part of \(F_{\text{REL}}\) in Eq. (9), is attributed to (r3) and (r3’) by Martynenko and Borie, respectively.

TABLE II. The item (r3’), remaining \((Z\alpha)^6\) corrections to finite size from Tab. 10 in meV, evaluated for an exponential and a uniform charge distribution of the deuteron, using the formulas given by Borie [22] p. 30, and Martynenko [24] Eq. (33), and the moments from Friar [46] Tab. V. For details, see text. Our average, \(\Delta E(r3’) = 0.0030(6)\) meV, is obtained from the spread of these values.

| Distribution   | after Borie [22] | after Martynenko [24] |
|----------------|------------------|-----------------------|
| Exponential    | 0.00238          | 0.00285               |
| Uniform        | 0.00350          | 0.00355               |

\[\langle r^3 \rangle_{(2)}\] has been coined “third Zemach moment” by Friar [46]. To avoid confusion with the “Zemach radius” \(r_Z\) that appears in the finite size effect in the 2S hyperfine splitting (Sec. IV C) we adopt the term “Friar moment” as recently suggested by Karshenboim [54].

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See e.g. Ref. [46] Eq. (43) or Ref. [22] p. 30.
TABLE III. Coefficients of the radius-dependent contributions to the Lamb shift. Values are in meV/fm$^2$, except for r3’. KS: Källén-Sabry, VP: vacuum polarization, SOPT: second-order perturbation theory.

| Contribution                        | Martynenko | Borie | Karshenboim | Our choice value source |
|------------------------------------|------------|-------|-------------|-------------------------|
| r1 Leading fin. size corr., (Zα)$^4$ | -6.07313 (27) | -6.0730 $b_a$ | -6.0732 $\Delta E_{FNS}^{(0)}$ | -6.07310 ±0.00010 avg. |
| r2 Radiative corr., α(Zα)$^5$      | -0.000962 $^c$ (62), [23] | -0.00072 $^c$ | -0.000962 | M                      |
| r3 Finite size corr. order (Zα)$^6$ | -0.002128 (33) | -0.00212 $b_c$ | -0.002124 ±0.000004 avg. |                      |
| r4 Uehling corr. (+KS), α(Zα)$^4$  | -0.01350 (28) | -0.0130 $b_d$ | -0.01325 ±0.00025 avg. |                      |
| r5 One-loop VP in SOPT, α(Zα)$^4$  | -0.020487 (29) | -0.02062 $b_c$ | -0.020554 ±0.000067 avg. |                      |
| r6 Two-loop VP corr., α$^2$(Zα)$^4$| -0.000105 (30, 31) | -0.000105 | -0.000105 | M                      |
| r7 Two-loop VP in SOPT, α$^2$(Zα)$^4$| -0.000095 (32) | -0.000095 | -0.000095 | M                      |
| r8 Corr. to the 2P$_{1/2}$ level    | -0.0000606 (b2p$_{1/2}$) | -0.0000606 (b2p$_{1/2}$) | +0.0000606 $^e$ | B                      |
| Sum                                | -6.10848 | -6.10952 $^d$ | -6.11025(28) | +0.00300(60) meV Tab. II |

| r3’ Remaining order (Zα)$^6$ [meV] $^c$ | 0.0029 meV (33) | 0.0033 meV | 0.00300 ±0.00060 meV Tab. II |
| Sum                                | -6.10848 $r_d^2$ + 0.0029 meV | -6.10952 $r_d^2$ + 0.0033 meV | -6.11025(28) $r_d^2$ + 0.00300(60) meV |

* This value was published with a wrong sign in [23]. The term is from Eq. (9) in [67].
* This value is obtained in [57], Eq. (10). For further explanations see Sec. III B.
* The sign is explained in the text.
* The $(r^2)$ coefficient given in Ref. [22] page 13, neglects the correction to the 2P$_{1/2}$ level, item (r8).
* Belongs to r3’. Depends on the charge distribution in a non-trivial way, see text.

We calculate (r3’) from Borie’s and Martynenko’s formula, for both an exponential and a uniform charge distribution, using the moments given by Friar [46] and obtain the values listed in Tab. II. We adopt the average, $\Delta E(r3’) = 0.0030(6)$ meV.

The items (r4) and (r5) do not depend on the shape of the deuteron charge distribution [22, 39]. The two-loop vacuum polarization corrections (r6) and (r7) are only given by Martynenko [24].

A correction to the 2P$_{1/2}$ level (r8) is given by Borie [22]. Item (r8) shifts the 2P$_{1/2}$ level “upwards” (less bound). This increases the energy difference between the 2S and 2P$_{1/2}$ levels, which explains the positive sign of this contribution in Tab. III. At the same time, this term decreases the fine structure (2P$_{3/2}$ − 2P$_{1/2}$ energy difference) and is hence listed as item (f10) with a negative sign in Tab. VI.

The total radius-dependent contribution to the Lamb shift yields

$$\Delta E_{rad.-dep.} = -6.11025(28) r_d^2 \text{ meV/fm}^2 + 0.00300(60) \text{ meV}. \tag{10}$$
C. Nuclear polarizability contributions to the Lamb shift

Historically, the two-photon exchange (TPE) contribution to the Lamb shift (LS) in muonic atoms has been considered the sum of the two parts displayed in Fig. 13 (a,b) and (c,d), respectively:

\[ \Delta E_{\text{TPE}} = \Delta E_{\text{Friar}}^{\text{LS}} + \Delta E_{\text{inelastic}}^{\text{LS}} \tag{11} \]

The elastic “Friar moment” contribution, \( \Delta E_{\text{Friar}}^{\text{LS}} \), also known as “third Zemach moment” \( \langle r^3 \rangle_{(2)} \) contribution, shown in Fig. 13(a,b) is sensitive to the shape of the nuclear charge distribution, beyond the leading \( \langle r^2 \rangle \) dependence discussed in Sec. IIIB. This part is traditionally parameterized as being proportional to the third power of the rms charge radius. The coefficient depends on the assumed radial charge distribution. For example, Borie gives \( \langle r^3 \rangle_{(2)} = 4.0(2) r^3 \), where \( r = \sqrt{\langle r^2 \rangle} \). For \( \mu d \), the Friar (3rd Zemach) moment contribution amounts to \( \sim 0.43 \text{ meV} \) \cite{62}.

The inelastic part, \( \Delta E_{\text{inelastic}}^{\text{LS}} \), frequently termed “nuclear polarizability contribution” is shown in Fig. 13(c,d). It stems from virtual excitations of the nucleus due to the exchange of two photons with the muon. The inelastic contributions are notoriously the least well-known theoretical contributions and limit the extraction of the charge radius from laser spectroscopy of the Lamb shift.

Early calculations of the contribution from the deuteron polarizability, i.e. the inelastic part \( \Delta E_{\text{inelastic}}^{\text{LS}} \) displayed in Fig. 13(c,d) include Fukushima et al. \cite{61}, 1.24 meV, Lu and Rosenfelder \cite{62}, 1.45 ± 0.06 meV, and Leidemann and Rosenfelder \cite{63}, 1.500 ± 0.025 meV. The latter value has been used extensively in the literature.

1. Modern determinations of \( \Delta E_{\text{TPE}}^{\text{LS}} \)

Recently, several works have revisited the TPE contributions to the Lamb shift in \( \mu d \). Tab. IV lists the contributions to \( \Delta E_{\text{TPE}}^{\text{LS}} \) obtained by Pachucki (2011) \cite{55}, Friar (2013) \cite{60}, Carlson et al. (2014) \cite{64}, the TRIUMF/Hebrew University group in Hernandez et al. (2014) \cite{58}, and Pachucki and Wienczek (2015) \cite{65}.

As it will turn out that the uncertainty in \( \Delta E_{\text{TPE}}^{\text{LS}} \) is by far the largest uncertainty in the determination of \( r_d \) from the \( \mu d \) data, we next summarize the main features of these papers. We identify missing and incorrect terms in the original papers. The detailed compilation in Tab. IV allows us to obtain the reliable average given in Eq. (17).

In his 2011 paper \cite{55}, Pachucki calculated the nuclear structure corrections to the Lamb shift in muonic deuterium using the AV18 potential for the deuteron and obtained \( \Delta E_{\text{TPE}}^{\text{LS}} = 1.680(16) \text{ meV} \). Moreover, he confirmed that for \( \mu d \), similar to electronic deuterium \cite{59, 60}, the elastic “Friar moment” contribution of order \( (Z\alpha)^5 \), \( \Delta E_{\text{Friar}}^{\text{LS}} \) (Fig. 13(a,b)) is canceled by a part of the inelastic two-photon (polarizability) contributions, \( \Delta E_{\text{inelastic}}^{\text{LS}} \) (Fig. 13(c,d)). The reason for this cancellation is that the deuteron binding energy of 2.2 MeV is small compared to the muon mass \cite{66}.

Pachucki \cite{55} includes both the elastic and inelastic TPE contribution of the proton, but not the neutron. For the proton, he rescaled the full proton TPE contribution calculated for muonic hydrogen \cite{60}, \( \Delta E(2S) = -0.0369(24) \text{ meV} \), with a reduced mass ratio to correct for the larger wave function overlap in \( \mu d \),

\[ \zeta = (m_{\mu d}^p / m_{\mu p}^p)^3 = 1.1685. \tag{12} \]

This gives a value of 0.043(3) meV for our items p13+p14. Pachucki’s value for the magnetic contribution (p10) was

\[ \Delta E_{\text{magnetic}} = 0.013(2) \text{ meV}. \]

For muonic hydrogen, in contrast, the first excited state of the nucleus (proton) is the \( \Delta \) resonance with an excitation energy of 300 MeV. Hence there is no such cancellation between elastic and inelastic TPE contributions in \( \mu p \).
found to be wrong by a factor of two in Ref. [58] and was corrected in Pachucki’s later work [65].

Friar (2013) used the zero-range approximation (ZRA) [61] which allows for a systematic derivation of all terms. Friar finds very good agreement with the results of Pachucki [55] despite the simplicity of the ZRA. The cancellation between elastic and inelastic TPE contributions is observed in ZRA, too 7 Friar noted that a nucleon finite size contribution of 0.028(2) meV should be added that had not been included in Ref. [55]. Friar’s value of \( \Delta E_{\text{LO-TPE}} = 1.941 \pm 0.015 \) meV seems at first glance to be in serious disagreement with Pachucki’s value [55].

The difference is however mainly caused by the Coulomb distortion (p5+p6) of \(-0.263\) meV which should be included in every calculation [67]. Including further items in Tab. [IV] like the nucleon polarizability contribution p14+p15, and the nucleon subtraction term p16 results in a “corrected value” of 1.697 meV. Higher order corrections to the dipole contribution (p3 and p4) can account for the remaining difference to the other model calculations to the dipole contribution (p3 and p4) can account for the remaining difference to the other model calculations and “our avg.”.

In their 2014 paper [58] the TRIUMF/Hebrew University group performed an independent calculation using two parameterizations of the deuteron potential: AV18 one the one hand, and nucleon-nucleon (NN) forces from chiral effective field theory (χEFT) up to order NLO-EGM and with various cutoffs, on the other. As in their work on muonic helium-4 [68, 69] they added higher order relativistic corrections, corrected the magnetic term, and added the intrinsic neutron polarizability [70]. They also introduced the reduced-mass-dependence in higher-order terms, while the earlier Ref. [55] had worked in the limit of infinite nuclear mass for all terms. The nuclear mass dependence for all terms was then further refined in Ref. [55].

Ref. [58] observed the cancellation of elastic and inelastic contribution for the muonic deuterium case explicitly: The sum of terms \( \delta^{(1)}_{Z1} + \delta^{(1)}_{Z3} = -0.424(3) \) meV in Ref. [58] cancels very nicely with elastic Friar (“3rd Zemach”) contribution \( \Delta E_{\text{LO-TPE}}^{\text{LS}} = 0.433(21) \) meV of the deuteron as calculated by Borie, see Ref. [22] p. 7.

Averaging over their results from AV18 and N3LO they obtained a value of \( \Delta E_{\text{LO-TPE}}^{\text{LS}} = 1.690(20) \) meV. The apparently good agreement with Pachucki’s value [55] may however be accidental as it arises from the cancellation of many small differences [58, 70]. Again, adding omitted items (p13 and p16) results in very good agreement with all other sums in Tab. [IV] Note that the 4th column in our Tab. [IV] (“Source 4”) is that value from Tab. 3 of Ref. [58], columns “N³LO-EM” and “N³LO-EGM”, which deviates most from their AV18 result. This is an attempt to be rather conservative when determining “our average” following Eq. (6). According to Bacca [70], their values for \( \delta^{(2)}_{N_S} \) (our item p11) should be updated to +0.020 meV from the published value of +0.015 meV [58].

The 2015 paper by Pachucki and Wienczek [65] updated Pachucki’s results from 2011 (Ref. [55]), again using the AV18 potential. Among other things, they included the finite size of the nucleons, and the intrinsic elastic and inelastic two-photon exchange with individual nucleons. They corrected their magnetic interaction term, and derived the correct mass dependence of the TPE correction and its consistent separation with the so-called pure recoil correction. Their total TPE contribution of order \( (Z\alpha)^5 \) is \( 1.717 \pm 0.020 \) meV. Item p16 must be added to obtain a “corrected value” in very good agreement with all other determinations.

Complementary to the calculations using various deuteron potentials [55, 58, 60, 65], Carlson et al. [64], in 2014, determined the TPE contributions with minimal model dependence using measured elastic and inelastic electron-deuteron scattering data and dispersion relations. Their model-independent calculation yields 2.01(74) meV, confirming the numbers given by [55, 58, 60] albeit with a much larger uncertainty. This uncertainty stems from the uncertainty in the data and can be improved significantly when new data from the Mainz MAMI and MESA facilities becomes available [64].

The several contributions to their sum can not be easily equated with individual items p1…p16 listed in Tab. [IV] so we do not quote their individual contributions, with one important exception. Carlson et al. [64] note that the proton and neutron intrinsic polarizabilities of 0.028(2) meV (our items p14+p15) should be added to the earlier results of Pachucki [55] and Friar [60]. Such a correction is already included in the later paper by Hernandez et al. [58].

On the other hand, the value of Carlson et al. [64] should be corrected [67, 69] for Coulomb distortion (p5+p6) of \(-0.263\) meV. Then the central value becomes 1.748 meV, in even better agreement with the (corrected) values from
nuclear models [55, 68, 60, 63]. Note that this correction corresponds to 1/3 of their quoted uncertainty and may hence look absurd. But the uncertainty quoted in Ref. [64] originates almost exclusively from the plain wave Born approx. (PWBA) term and may be reduced by at least a factor of 4 with new data from a planned experiment in Mainz [64]. The good agreement between the corrected central value and all other (corrected) values makes one wonder if the uncertainty in Ref. [64] is maybe somewhat conservative.

The “Thomson term” is a recoil correction that has first been calculated in Ref. [61]. It has received some attention [47, 67, 70, 71] in the discussion of our Tab. IV and the conclusion was that this term is indeed correctly added to the sum of the contributions in the dispersion-relation treatment of Ref. [61]. The other calculations [55, 68, 60, 66] have correctly not included such a term, because the cancellation between elastic and (part of the) inelastic contributions to the polarizability will eliminate this Thomson term (as well as other similar recoil-like terms) in such a “nuclear Hamiltonian approach”. All further recoil corrections of order ($Z\alpha$) to the Lamb shift in muonic deuterium are then included in the “pure recoil corrections”, item #22 in Tab. I.

2. Comparison of terms and further corrections

An earlier version of the present manuscript was sent to the authors of Refs. [55, 58, 60, 64, 65] and other experts in the field. The ensuing insightful discussions resolved several discrepancies between the published values of $\Delta E^{LS}_{TPE}$ and revealed that some further corrections should be included.

Table IV lists in chronological order the modern determinations of $\Delta E^{LS}_{TPE}$ using various nuclear models, and scattering data. As usual, we calculate an “average” following our Eq. (6) and consider the spread of values in the uncertainty.

Items p1 through p10 contain the nuclear contributions, and the various calculations are in good agreement.

It is satisfying to note that the dominant dipole term, item p1, is in very good agreement for the three models used: AV18, ZRA, and $N^3$LO χEFT. We average the results using “modern” potentials [55, 65] and take the agreement of the ZRA result as an indication that the ZRA results for the smaller terms are likely to be accurate on the few $\mu$eV level and can hence be used in “our average”.

Items p2..p4 are relativistic corrections to p1. The two most recent works [58, 65] include higher order relativistic corrections so we consider only these works in the average.

There is consensus that the Coulomb distortion contribution (p5+p6) should be included in all calculations. Adding our average of -0.263 meV to the results of Friar [60] and Carlson et al. [64] removes most of the discrepancy between all published values.

Nuclear excitation corrections p7..p9 cancel to some degree. Our average includes the results from ZRA [60] and the most recent AV18 and $N^3$LO models [58, 65].

The magnetic contribution p10 from Ref. 55 has been corrected in the later work 65. We average over all the other results.

Items p11 through p16 are the nucleon contributions.

Item p11 from the TRIUMF/Hebrew University group ($\delta^{(2)}_{NS}$ in Ref. [55]) has been updated to to +0.020 meV [70], further improving the agreement with Refs. [60, 65].

After some discussions, consensus has been reached that several nucleon contributions should be included [47, 67, 71, 72]: The elastic Friar (3rd Zemach) term of the proton (p13), the inelastic proton and neutron contributions (p14+p15), and the subtraction terms from both the proton and the neutron (p16) are therefore included in our sum. In principle, the elastic Friar term of the neutron should be included too, but it is small enough to be neglected [60, 65, 71].

We follow the suggestion of Birse and McGovern [71] who obtain these values as follows:

Item p13, the elastic Friar (3rd Zemach) moment contribution of the proton to the Lamb shift in $\mu d$ is obtained from the values of the elastic and the non-pole Born term calculated for muonic hydrogen ($\mu p$) [71].

Both, the elastic term in $\mu p$, and the non-pole term in $\mu p$, have been obtained by Carlson and Vanderhaeghen from scattering data using dispersion relations [66]. Their value for the elastic term, $\Delta E^{3l}$, amounts to 0.0295 ± 0.0013 meV [7]. Their value for the non-pole Born term for $\mu p$ is $-0.0048$ meV [7]. The sum of these two terms, rescaled with $\zeta$ from Eq. (12) yields for p13, the elastic Friar moment contribution of the proton to the Lamb

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9 The sign convention in Ref. [66] is opposite to the one used here.
shift in muonic deuterium, the value
\[ \Delta E_{\text{Friar}}^{\text{LS}}(p) = 0.0289 \pm 0.0015 \text{ meV}. \] (13)

The inelastic proton and neutron polarizabilities \( p_{14} \) and \( p_{15} \) have been calculated from deuteron data and dispersion relations by Carlson et al. [64]. Their result for the sum \( p_{14}+p_{15} \) amounts to
\[ \Delta E_{\text{inelastic}}^{\text{LS}}(p) + \Delta E_{\text{inelastic}}^{\text{LS}}(n) = 0.028 \pm 0.002 \text{ meV} \] (14)
which is the value we adopt. Hernandez et al. [58] used the value 0.027(2) meV from the same Ref. [64]. This number is, however, only an estimate using numbers rescaled from muonic hydrogen, whereas our choice Eq. (14) is calculated from deuteron data, and the value in Eq. (14) should be used [67].

Finally, the contribution from the “subtraction term” of the nucleon polarizabilities has to be considered, too [67, 71]. Birse and McGovern have calculated the subtraction term for the inelastic TPE of the proton in muonic hydrogen, \( \Delta E_{\text{sub}} = -0.0042 \pm 0.0010 \text{ meV} \) [72] using chiral perturbation theory. This value is in good agreement with the value \( \Delta E_{\text{sub}}^{\text{b}} = -0.0053 \pm 0.0019 \text{ meV} \) [73] from Carlson and Vanderhaeghen [60] which was however obtained from a particular model of the proton form factor and an older value of the proton magnetic polarizability [71]. For the deuteron, we hence adopt the former value, double it assuming that the proton and neutron contributions are approximately the same [71], and rescale with \( \zeta \) from Eq. (12) to yield \( p_{16} \) for muonic deuterium
\[ \Delta E_{\text{sub}}^{\text{LS}}(p) + \Delta E_{\text{sub}}^{\text{LS}}(n) = -0.0098 \pm 0.0098 \text{ meV}. \] (15)
Here we have assigned a 100% uncertainty.

3. Our choice

Summing all values in Tab. IV and adding the uncertainties from (the spreads of) our averaging in quadrature, gives
\[ \Delta E_{\text{TPE}}^{\text{LS}}(\text{simple}) = 1.7091 \pm 0.0146 \text{ meV}. \] (16)
This uncertainty is smaller than the published uncertainties in all original papers [55, 58, 60, 64, 65]. Hence we increase conservatively the uncertainty in our average to the 0.020 meV obtained by the two most recent model calculations [58, 65].

The total TPE contribution of order \((Z\alpha)^5\) to the Lamb shift in muonic deuterium [\textsuperscript{11}] is hence
\[ \Delta E_{\text{TPE}}^{\text{LS}}(\text{final}) = 1.7091 \pm 0.0200 \text{ meV}. \] (17)
Further rounding is deferred to Eq. (18).

The uncertainty of the TPE contribution is by far the dominant one, and it limits severely the accuracy of the deuteron rms charge radius obtained from laser spectroscopy of the Lamb shift in muonic deuterium.

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\[ ^{10}\text{The sign convention in Ref. [73] is opposite to the one used here.} \]

\[ ^{11}\text{Note that non-perturbative Coulomb corrections of higher order in } (Z\alpha) \text{ have been accounted here, whereas the pure recoil part of the TPE has been separately given in Tab. [\#22].} \]
TABLE IV. Deuteron structure contributions to the Lamb shift in muonic deuterium. Values are in meV. For source 4, the N3LO† calculation by Hernandez et al. we use their value from the rightmost two columns of their Tab. 3 that differs most from their “AV18” value. Items with a diamond † are corrected from the published values, see footnotes.

| Item          | Contribution                                      | Pachucki [53] AV18 | ZRA         | Hernandez et al. [58] N3LO† | Pach. & Wienczek [55] AV18 | Carlson et al. [61] | Our choice data | source |
|---------------|---------------------------------------------------|--------------------|-------------|-----------------------------|-----------------------------|---------------------|----------------|--------|
| Source        |                                                   | 1                  | 2          | 3                          | 4                           | 5                   | 6               |        |
| p1            | Dipole                                           | 1.910 δ₂E         | 1.925       | Leading C1                 | 1.907 1.926 0.026 δ₂E       | 1.910 δ₂E           | 1.9165 ± 0.0095 | 3-5    |
| p2            | Rel. corr. to p1, longitudinal part               | −0.035 δₚE        | −0.037      | Subleading C1              | −0.029 −0.030 0.026 δₚE    | −0.026 δₚE         |                 |        |
| p3            | Rel. corr. to p1, transverse part                 | 0.012 0.013       | 0.024       |                            | 0.004 0.022               | 0.022               |                 |        |
| p4            | Rel. corr. to p1, higher order                    |                     |             |                            | 0.017 −0.017              | −0.0195 ± 0.0025   |                 |        |
| sum           | Total rel. corr., p2+p3+p4                       | −0.035 −0.037      | −0.017      |                            | 0.017 −0.017              |                    |                 | 3-5    |
| p5            | Coulomb distortion, leading                      | −0.255 δ₃₁E       | −0.262 −0.264 | 0.324 δ₃₂E                 | −0.255 δ₃₁E               | −0.006 δ₃₂E        |                 |        |
| p6            | Coul. distortion, next order                     | −0.006 δ₃₂E       | 0.034 C0 + ret-C1 + C2   | 0.036 0.038               | 0.036                      | 0.036               |                 | 2-5    |
| sum           | Total Coulomb distortion, p5+p6                  | −0.261             | 0.040       |                            | 0.040                      | 0.036               |                 | 2-5    |
| p7            | El. monopole excitation                          | −0.045 δ₆₀E       | −0.042 C0   |                            | 0.042 δ₆₀E                | −0.042 δ₆₀E        |                 | 3-5    |
| p8            | El. dipole excitation                            | 0.151 δ₄₁E        | 0.137 Retarded C1        | 0.139 0.140 0.139 δ₄₁E    | 0.139 δ₄₁E            | 0.139 δ₄₁E        |                 |        |
| p9            | El. quadrupole excitation                        | −0.066 δ₆₂E       | −0.061 C2   |                            | −0.061 δ₆₂E               | −0.061 δ₆₂E        |                 | 3-5    |
| sum           | Tot. nuclear excitation, p7+p8+p9                | 0.040              | 0.034 C0 + ret-C1 + C2   | 0.036 0.038               | 0.036                      | 0.036               |                 | 2-5    |
| p10           | Magnetic                                         | −0.008 −0.011 M1   | −0.008 −0.007 δ₉₀δ₉₀E    | −0.008 δ₉₀δ₉₀E           | −0.008 δ₉₀δ₉₀E       | −0.0090 ± 0.0020  |                 | 2-5    |
| SUM1          | Total nuclear (corrected)                        | 1.646              | 1.648       |                            | 1.656                      | 1.676               | 1.6615 ± 0.0103 |        |
| p11           | Finite nucleon size                              | 0.021 Retarded C1 f.s. | 0.020 δ₉₀δ₉₀E    | 0.020 δ₉₀δ₉₀E           | 0.020 δ₉₀δ₉₀E       | 0.020 δ₉₀δ₉₀E      |                 |        |
| p12           | n p charge correlation                           | −0.023 pn correl. f.s. | −0.017 −0.017 δ₉₀δ₉₀E | −0.018 δ₉₀δ₉₀E           | −0.018 δ₉₀δ₉₀E       | −0.018 δ₉₀δ₉₀E     |                 |        |
| sum           | p11+p12                                          | −0.002             | 0.003 0.003       |                            | 0.002                      | 0.002               | 0.0005 ± 0.0025 | 2-5    |
| p13           | Proton elastic 3rd Zemach moment                 | 0.043(3) δ₇E       | 0.030 r₃₉p₆₈(2)       | 0.027(2) δ₉₀δ₉₀E         | 0.043(3) δ₇E            | 0.043(3) δ₇E       | 0.0289 ± 0.0015 | Eq. 13a |
| p14           | Proton inelastic polarizab.                      |                   | 0.030 r₃₉p₆₈(2)       | 0.027(2) δ₉₀δ₉₀E         | 0.043(3) δ₇E            | 0.043(3) δ₇E       | 0.0280 ± 0.0020 | 6      |
| p15           | Neutron inelastic polarizab.                     |                   | 0.030 r₃₉p₆₈(2)       | 0.027(2) δ₉₀δ₉₀E         | 0.043(3) δ₇E            | 0.043(3) δ₇E       | 0.0280 ± 0.0020 | 6      |
| p16           | Proton & neutron subtraction term                |                   | 0.030 r₃₉p₆₈(2)       | 0.027(2) δ₉₀δ₉₀E         | 0.043(3) δ₇E            | 0.043(3) δ₇E       | 0.0280 ± 0.0020 | 6      |
| sum           | Nucleon TPE, p13+p14+p15+p16                     | 0.043(3)           | 0.030 r₃₉p₆₈(2)       | 0.027(2) δ₉₀δ₉₀E         | 0.043(3) δ₇E            | 0.043(3) δ₇E       | 0.0280 ± 0.0020 | 6      |
| SUM2          | Total nucleon contrib.                           | 0.043(3)           | 0.028 r₃₉p₆₈(2)       | 0.027(2) δ₉₀δ₉₀E         | 0.043(3) δ₇E            | 0.043(3) δ₇E       | 0.0280 ± 0.0020 | 6      |
| Sum, published |                                                   | 1.680(16)          | 1.941(19)       | 1.690(20)                 | 1.717(20)                | 2.011(740)         | 1.7091 ± 0.0146 |        |
| Sum, corrected |                                                   | 1.697(19)          | 1.714(20)       | 1.707(20)                 | 1.748(740)               | 1.7091 ± 0.0146    |                 |        |

a Corrected from -0.016 meV, see Ref. [63] below Eq. (45).

b The Coulomb distortion contribution p5+p6 of -0.263 meV (our choice) has been added to Friar’s sum of 1.911 meV to make the numbers comparable.

c Corrected from +0.015 meV [70].

d Rescaled from the muonic hydrogen values from Refs. [69] [73]. See text.

e Rescaled from the muonic hydrogen value from Ref. [73]. See text.

f See text.

g Corrections: p5+p6, p14+p15+p16. Items p3+p4 (higher order corr. to p1) would increase this value by another ~ 0.015 meV.

h Corrections: p13, p16. Item p11 updated from 0.015 meV [63].

i Correction: p16.

j Correction: p5+p6.
D. Total Lamb shift in muonic deuterium

Collecting the radius-independent (mostly) QED contributions listed in Tab. I and summarized in Eq. (8), the radius-dependent contributions listed in Tab. III and summarized in Eq. (10), and the complete two-photon (polarizability) contribution $\Delta E_{\text{TPE}}^{\text{LS}}$ from Eq. (17), we obtain for the $2S - 2P$ energy difference in muonic deuterium

$$ΔE(2S - 2P_{1/2}) = 228.77356(75) \text{ meV}$$

$$+ 0.00300(60) \text{ meV} - 6.11025(28) r_d^2 \text{ meV/fm}^2$$

$$+ 1.70910(2000) \text{ meV}$$

$$= 230.486(20) \text{ meV} - 6.1103(3) r_d^2 \text{ meV/fm}^2$$

(18)

where in the last step we have rounded the values to reasonable accuracies.

One should note that the uncertainty of 0.020 meV from the nuclear structure corrections $\Delta E_{\text{TPE}}^{\text{LS}}$, Eq. (17), is about 30 times larger than the combined uncertainty of all radius-independent terms summarized in Tab. I and 15 times larger than the uncertainty in the $\langle r^2 \rangle$ coefficient (which amounts to 0.0013 meV). A further improvement of the nuclear structure corrections in light muonic atoms is therefore desirable.

IV. 2S HYPERFINE SPLITTING

A. Fermi and Breit contributions

The interaction between the magnetic moment of the nucleus with the magnetic field induced by the lepton gives rise to shifts and splittings of the energy levels termed hyperfine effects. In classical electrodynamics, the interaction between the magnetic moments $\mu_d$ and $\mu_\mu$ of deuteron and muon, respectively, is described by

$$H_{\text{HFS}}^{\text{classical}} = -\frac{2}{3} \mu_d \cdot \mu_\mu \delta(r)$$

(19)

where $\delta(r)$ is the delta-function in coordinate space. A similar Hamiltonian to the one in Eq. (19) can be derived in quantum field theory from the one-photon exchange diagram. Using the Coulomb wave function, this gives rise in first-order perturbation theory to an energy shift the radius-dependent contributions listed in Tab. III and summarized in Eq. (10), and the complete two-photon (polarizability) contribution $\Delta E_{\text{TPE}}^{\text{LS}}$ from Eq. (17), we obtain for the $2S - 2P$ energy difference in muonic deuterium

$$\Delta E_{\text{HFS}}(F) = \frac{4(Z\alpha)^4 m_d^3}{3n^3 m_\mu m_d} (1 + \kappa)(1 + a_\mu) \frac{1}{2} \left[ F(F+1) - \frac{11}{4} \right]$$

$$= \frac{1}{3} \Delta E_{\text{Fermi}} \left[ F(F+1) - \frac{11}{4} \right]$$

(20)

where $\Delta E_{\text{Fermi}}$ is the Fermi splitting, $m_d$ is the deuteron mass, $F$ is the total angular momentum, $\kappa$ and $a_\mu$ are the deuteron and muon anomalous magnetic moments, respectively.

The Fermi splitting

$$\Delta E_{\text{Fermi}} = \frac{2(Z\alpha)^4 m_d^3}{3n^3 m_\mu m_d} (1 + \kappa)(1 + a_\mu)$$

$$= \frac{3}{2} \beta_D(1 + a_\mu)$$

(21)

with

$$\beta_D = \frac{4(Z\alpha)^4 m_d^3}{3n^3 m_\mu m_d} (1 + \kappa)$$

(22)

is the main contribution to the HFS, (h1) in Tab. V. The value Borie gives on p. 19 of Ref. [22] is

$$\Delta E_{\text{Fermi}}^{\text{B}} = 6.14298 \text{ meV}.$$  

(23)

It already includes the correction $\Delta E_{\mu\text{AMM}}$ (h4) due to the muon anomalous magnetic moment ($\mu$AMM). However, Borie’s value $\Delta E_{\text{Fermi}}^{\text{B}} = 6.14298 \text{ meV}$ is not correct. Since $\Delta E_{\text{Fermi}}$ depends only on fundamental constants [4], we have recalculated it following Eq. (21), and obtain a value of

$$\Delta E_{\text{Fermi}} = 6.14308 \text{ meV}$$

(24)

which differs from Borie’s, but coincides with Martyenenko’s value.
\[
\Delta E_{\text{Fermi}}^M = 6.1431 \text{ meV} \\
= 6.1359 \text{ meV}_{h1} + 0.0072 \text{ meV}_{h4}.
\] (25)

Here, the two terms in the second line are, respectively, the Fermi splitting excluding the contribution of the anomalous magnetic moment of the muon, \((h1)\), and the \(\mu\)AMM correction, \((h4)\), which Martynenko calculates separately.

The Breit term \(\Delta E_{\text{Breit}}\) \((h2)\) corrects for relativistic and binding effects accounted for in the Dirac-Coulomb wave function but excluded in the Schrödinger wave function. Both, Martynenko and Borie, calculated the Breit correction term to be

\[
\Delta E_{\text{Breit}} = 0.0007 \text{ meV}.
\] (26)

### B. Vacuum polarization (VP) and self-energy (SE) contributions

On p. 21 of Ref. [22], Borie provides the values for \(\epsilon_{\text{VP1}}\) \((h8)\) and \(\epsilon_{\text{VP2}}\) \((h9)\), for a point-like nucleus. In Sec. [IVC] we give a correction due to the finite size, which is given by \((h25, h26)\). The corresponding terms from Martynenko and Borie agree.

\((h7)\) is neglected by Martynenko as pointed out on p. 21 in [22]. The origin of the difference between Martynenko and Borie in \((h9b)\) is not clear. In this case we take the average. \((h9b)\) is a correction in third order perturbation theory which is only given by Martynenko.

The \(\mu\)VP contribution \(\Delta E_{\mu\text{VP}}\) \((h12)\) is given by Martynenko as

\[
\Delta E_{\mu\text{VP}} = 0.0002 \text{ meV}.
\] (27)

Borie included this contribution in the vertex term \(\Delta E_{\text{vertex}}\) \((h13)\) as pointed out on p. 21 in [22]. As we do not use Borie’s vertex term, we have to consider the \(\mu\)VP term from Martynenko.

Martynenko gives a value for a term called radiative nuclear finite size correction \((h17b)\). It is composed of four terms, \(\mu\text{SE with nuclear structure, jellyfish correction and two vertex correction terms, so it should also include } (h13)\). Their sum yields \(-0.0005 \text{ meV}\). We think that \((h14)\) is an additional term, only calculated by Borie. So we add this to ‘our choice’.

The hadron VP \(\Delta E_{h\text{VP}}\) \((h18)\) results equal for both, Martynenko and Borie:

\[
\Delta E_{h\text{VP}}^{M,B} = 0.0002 \text{ meV}.
\] (28)

There is no considerable contribution from weak interaction [74].

### C. Zemach radius

The Bohr-Weisskopf effect [25] is the main finite size correction to the 2S hyperfine splitting. It is also called the Zemach term [76]. \(\Delta E_{\text{Zemach}}^{\text{HFS}}\), and is listed as item \((h20)\) in our summary. The Zemach term is usually parameterized as [77]

\[
\Delta E_{\text{Zemach}}^{\text{HFS}} = -\Delta E_{\text{Fermi}} \cdot 2(Z\alpha)m_r r_Z\] (29)

using the so-called Zemach radius of the nucleus [77]

\[
r_Z = \int d^3r \int d^3r' \rho_E(r) \rho_M(r-r')
= -\frac{4}{\pi} \int_0^{\infty} dq \left( G_E(q^2) G_M(q^2) - 1 \right).\] (30)

This convolution of charge \(\rho_E(r)\) and magnetization \(\rho_M(r)\) distribution comes from the fact, that the finite charge distribution alters the muon’s wave function at the origin.

Diagrammatically, the Zemach correction \((h20)\) to the HFS, \(\Delta E_{\text{Zemach}}^{\text{HFS}}\), is the elastic part of the two-photon exchange contribution to the 2S HFS, just like the Friar correction to the Lamb shift Fig. 13(a,b) [18].

A recoil correction to the elastic TPE, \((h23)\), is considered here, too. It is somewhat parallel to the item \#22 of the Lamb shift, termed rel. RC \((Z\alpha)^5\) listed in Tab. [I].

The inelastic part of the TPE correction to the 2S HFS, \(\Delta E_{\text{inelastic}}^{\text{HFS}}\), is topic of the next Sec. [IVD].

Borie gives a value of \(\epsilon_{\text{Zemach}} = -0.007398 \text{ fm}^{-1} r_Z\) (Ref. [22], p. 22). Her Zemach contribution is hence (Eq. [29], Ref. [22], p. 23 top)

\[
\Delta E_{\text{Zemach}}^{\text{HFS}} \text{(Borie)} = -0.04545 r_Z \text{ meV/fm}.\] (31)

Note that the coefficient
\[
-0.04545 = 3 \frac{\beta_D}{2}(1 + a_\mu) \epsilon_{\text{Zemach}}\] (32)
does explicitly include the factor \((1 + a_\mu)\).

Using \(r_Z = 2.593 \pm 0.016 \text{ fm}\) from Ref. [77] Borie’s value for the Zemach contribution to the 2S HFS amounts to

\[
\Delta E_{\text{Zemach}}^{\text{HFS}} \text{(Borie)} = -0.11782 \pm 0.00074 \text{ meV}.\] (33)

Borie mentions that nuclear recoil corrections (our item \((h23)\)) are important, but have not been included (Ref [22], p. 22, bottom).
Martynenko calculates the nuclear structure correction $\alpha^5$ from the deuteron electromagnetic current that involves the form factors $F_1, F_2,$ and $F_3$ which can be related to the measured charge, magnetic and quadrupole form factors of the deuteron, $G_E(q^2), G_M(q^2)$ and $G_Q(q^2)$, see Eq. (37) in Ref. [15]. Using the parameterization of $G_E, G_M$ and $G_Q$ from Ref. [78], Martynenko obtains a value of $-0.1163 \pm 0.0010$ meV (Ref. [15], Tab. 1 item #7, Eq. (46)). This value is the sum of the Zemach term, item (h20), as calculated by Borie, but includes recoil corrections to the finite size effect, (h23) [33]. The separation of these two contributions is not unique [33], but if one adopts the canonical definition of the Zemach radius in terms of the form factors $G_E$ and $G_M$ as given in Eq. (30), one can separate Martynenko’s sum into

$$\Delta E_{Zemach+RC}^{\text{HFS}} (\text{Martynenko}) = -0.1163 \text{ meV} \pm 0.0010 \text{ meV} = (-0.1178 \text{ meV}_{h20} + 0.0015 \text{ meV}_{h23}) \pm 0.0010 \text{ meV}. \quad (34)$$

Here the item (h20) was calculated using the Zemach radius $r_Z = 2.5959$ fm [33], obtained by numerical integration of the parameterization of the deuteron form factors from Ref. [78]. This Zemach radius is in excellent agreement with the value $r_Z = 2.593 \pm 0.016$ fm from Ref. [77] used by Borie [22]. A small difference arises from Martynenko’s observation that the factor $(1 + a_\mu)$ in Eq. (21) should not be included for the $2\gamma$ amplitudes with point vertices [33].

Rewriting the $-0.1178$ meV of (h20) as

$$\Delta E_{Zemach}^{\text{HFS}} (\text{Martynenko}) = -0.0453934 \frac{r_Z \text{ meV}}{\text{fm}} \quad (35)$$

makes the dependence on the Zemach radius explicit. Putting the nuclear recoil corrections back in, the combined Zemach (h20) and recoil (h23) corrections evaluated by Martynenko (Eq. (34)) become

$$\Delta E_{Zemach+RC}^{\text{HFS}} = -0.0453934 r_Z \text{ meV/fm}_{h20} + (0.0015 \pm 0.0007) \text{ meV}_{h23} \quad (36)$$

which we adopt. The total uncertainty of 0.0010 meV given by Martynenko is then the sum of the uncertainty in the Zemach radius $\delta r_Z = 0.016$ fm, corresponding to 0.0007 meV, and the uncertainty of (h23) given above.

D. Nuclear polarizability contributions to the 2S HFS

The polarizability contribution to the 2S hyperfine splitting in muonic deuterium, $\Delta E_{\text{TPF}}^{\text{HFS}}$, has only recently been calculated for the first time by the group of Martynenko [15]. They obtain the polarizability term in two parts:

First, the deuteron polarizability contribution $\Delta E_{\text{TPF}}^{\text{HFS}}(\text{deuteron})$ (h22a) is obtained from the analytic expressions derived in zero range approximation for electronic deuterium by Khriplovich and Milstein [79]. This part takes into account the virtual excitation of a deuteron made from point nucleons.

Second, the much smaller internal deuteron polarizability contribution $\Delta E_{\text{int. d-pol.}}^{\text{HFS}}$ (h22b), which accounts for the excitation of the individual nucleons (proton and neutron) inside the deuteron. This part is estimated based on the results for muonic hydrogen [80].

Summing these two up yields

$$\Delta E_{\text{tot. d-pol.}}^{M} = 0.2121(42) \text{ meV} + 0.0105(25) \text{ meV} = 0.2226(49) \text{ meV} \quad (37)$$

with a generous uncertainty that accounts also for the fact that the original derivation [79] was for electronic,
and not for muonic deuterium.

Eq. (37) is also the value quoted by Borie. As pointed out by Borie, Ref. [22] p. 22, it is not clear whether the 'elastic' contribution of the two-photon exchange diagrams is taken into account.

As for the Lamb shift, the polarizability term for the 2S HFS is the one with by far the largest uncertainty.

E. Further corrections to the 2S HFS

Several further corrections are considered by either Martynenko or Borie (h24, h25, h26, h27, and h27b): Martynenko calculates a mixed term which includes eVP and a nuclear structure correction (h24)

\[ \Delta E_{\text{eVP+nucl.struct.}}^M = 0.0019 \text{ meV} \]  

(38)
as well as two further nuclear structure contributions (h27, h27b):

\[ \Delta E_{\text{nucl.str.corr.}}^M = 0.0008 \text{ meV} \]  

(39)

\[ \Delta E_{\text{nucl.str.SOFT}}^M = -0.0069 \text{ meV} \]  

(40)

Borie gives finite size corrections (h25, h26) to the eVP terms \( \epsilon_{\text{VP1}} \) and \( \epsilon_{\text{VP2}} \), both contributing -0.00068 meV. These are obtained by calculating the difference of \( \epsilon_{\text{VP1}} \) and \( \epsilon_{\text{VP2}} \) with a point size nucleus compared to the ones when considering a finite size ([22], p. 21). It is not yet clear whether the nuclear structure contributions from Martynenko are complementary to the ones of Borie. We should remark that item (h27b) is quite big. It doesn’t seem to be included in Borie’s calculations and is the main reason for the difference between Borie [22] and Martynenko [15].

For now we refrain from assigning a large uncertainty to this item h27b, but an independent calculation, or at least an estimate of it’s accuracy, would certainly be helpful.

F. Total 2S hyperfine splitting

Hence, collecting all terms, but separating out the deuteron polarizability correction Eq. (37) as it is the dominant source of uncertainty, we can write the total 2S HFS in muonic deuterium as

\[
\Delta E_{\text{HFS}}^{\text{th}} = 6.17415(73) \text{ meV} + 0.22260(490) \text{ meV} - 0.04539 r_Z \text{ meV} \\
= 6.39675(494) \text{ meV} - 0.04539 r_Z \text{ meV}
\]  

(41)

The large uncertainty in the polarizability corrections to the 2S HFS will prevent a determination of the deuteron Zemach radius from the measured transitions in muonic deuterium [10]. An improved calculation of the polarizability terms is therefore highly desirable.

Using the Zemach radius \( r_Z = (2.593 \pm 0.016) \text{ fm} \) [77] we get:

\[ \Delta E_{\text{HFS}}^{\text{th}} = 6.27905(495) \text{ meV} \]  

(42)

to be compared to the muonic deuterium measurement [10]. Alternatively, one can use the measurement and the Zemach radius to accurately determine the polarizability contributions. Such a number may serve as a benchmark for accurate lattice calculations.
TABLE V. All contributions to the 2S hyperfine splitting (HFS) in muonic deuterium. The item numbers hi in the first column follow the entries in Tab. 3 of Ref. [3]. For Martynenko, numbers #1 to #15 refer to rows in Tab. I of Ref. [15], whereas numbers in parentheses refer to equations therein. Borie [22] gives the values as coefficients to be multiplied with the sum of (h1+h4). We list the resulting values in meV. AMM: anomalous magnetic moment, PT: perturbation theory, VP: vacuum polarization, SOPT: second order perturbation theory, TOPT: third order perturbation theory.

All values are in meV (meV/fm for h20).

| Contribution | Martynenko [15] | Borie [22] | Our choice |
|--------------|-----------------|------------|-------------|
| h1 Fermi splitting, \((Z\alpha)^4\) | 6.1359 | #1, (6) | 6.14298 p. 19 | 6.14308 Eq. 24 |
| h4 \(\mu\)AMM corr., \(\alpha(Z\alpha)^4\) | 0.0072 | #2, (7) | 0.00069 | 0.00069 B |
| sum (h1+h4) | 6.1431 | 6.14298 p. 19 | 6.14308 Eq. 24 |
| h2 Breit corr., \((Z\alpha)^5\) | 0.0007 | #3, (8) | 0.00069 | 0.00069 B |
| h5 eVP in 2nd-order PT, \(\alpha(Z\alpha)^5\) (\(e_{VP2}\)) | 0.0207 | #4, (23) | 0.02070 p. 21 | 0.0207 M |
| h7 Two-loop corr. to Fermi-energy (\(e_{VP2}\)) | neglected | | 0.00016 p. 21 | 0.00016 B |
| h8 One-loop eVP in 1st int., \(\alpha(Z\alpha)^4\) (\(e_{VP1}\)) | 0.0134 | #4, (12) | 0.01339 p. 21 | 0.0134 M |
| h9 Two-loop eVP in 1st int., \(\alpha^2(Z\alpha)^4\) (\(e_{VP1}\)) | 0.0005 | #5, (16), (29-32) | 0.00010 p. 21 | 0.0003 ± 0.0002 avg. |
| h9b VP corr. in TOPT | 0.00004 | #6, (33) | 0.00004 | |
| h12 \(\mu\)VP (sim. to \(e_{VP}\)) | 0.0002 | #9, (48) | 0.0002 | 0.0002 B |
| h13 Vertex, \(\alpha(Z\alpha)^5\) incl. in h17b | | | | |
| h14 Higher order corr. of (h13), part with \(ln(\alpha)\) | | | | |
| h17b Radiative nucl. fin. size corr., \(\alpha(Z\alpha)^5\) | -0.0005 | #13, (71-74) | | |
| h18 Hadron VP, \(\alpha^6\) | 0.0002 | #10, (50) | 0.00016 | 0.00016 B |
| h19 Weak interact. corr. | 0 | p. 10 | 0.0016 | 0.00016 |
| h20 Fin. size (Zemach) corr. to \(\Delta E_{\text{Fermi}}, (Z\alpha)^5\) | -0.04539 \(r_Z\) | \(33^\circ\) | -0.04545 \(r_Z\) | 0.04539 \(r_Z\) M |
| h23 Recoil corr. to fin. size | 0.0015 | ± 0.0007 | \(33^\circ\) | 0.0015 | ± 0.0007 M |
| sum (h20+h23) | -0.1163 | ± 0.0010 | #7, (46) | 0.0015 | ± 0.0007 M |
| h22a Deuteron polarizability, \((Z\alpha)^5\) | 0.2121 | ± 0.0042 | #14 using \(79\) | 0.2121 | ± 0.0042 M |
| h22b Deuteron internal polarizability, \((Z\alpha)^5\) | 0.0105 | ± 0.0025 | #15 using \(80\) | 0.0105 | ± 0.0025 M |
| sum (h22a+h22b) | 0.2226 | ± 0.0049 | 0.2226 | ± 0.0049 p. 22 | 0.2226 | ± 0.0049 p. 22 |
| h24 eVP + nucl. struct. corr., \(\alpha^6\) | 0.0019 | ± 0.00001 | #8, (47) | | 0.0019 | |
| h25 eVP corr. to fin. size (sim. to \(e_{VP2}\)) | | | | | | |
| h26 eVP corr. to fin. size (sim. to \(e_{VP1}\)) | | | | | | |
| h27 Nucl. struct. corr., \((Z\alpha)^5\) | 0.0008 | #11, (55) | 0.0008 | M |
| h27b Nucl. struct. in SOPT | -0.0069 | #12, (59) | | | -0.0069 M |

| Sum | 6.39824 ± 0.00494 | 6.39880 ± 0.00490 | 6.39675 ± 0.00494 | -0.04539 \(r_Z\) |

a The published value for the sum of items h20+h23 is \(-0.1163 ± 0.0010\) meV [15]. For the separation into items h20 and h23 see text.

b Calculated from Eq. (21), including the factor \((1 + a_\mu)\). According to Martynenko, this factor should be omitted in the 2\(\gamma\) amplitudes with point vertices.

c Difference of two terms in Borie [22]. See text.
TABLE VI. Contributions to the 2P fine structure. The items (f7a), (f7d), and (f7e) originate from the same graphs as the Lamb shift items #11, #12, and #30*, respectively. VP: vacuum polarization, AMM: anomalous magnetic moment, KS: Källén-Sabry.

All values are in meV.

| Contribution | Martynenko 23 Tab.2 | Borie 22 | Karshenboim 24 Tab.IV | Our choice |
|--------------|----------------------|---------|-----------------------|------------|
| f1 Dirac     |                      |         | 8.86430               |            |
| f2 Recoil    |                      |         | −0.02521              |            |
| f3 Contrib. of order \((Z\alpha)^4\) | 8.83848 |         | 8.83909               |            |
| f4 Contrib. of order \((Z\alpha)^6\) and \((Z\alpha)^6\) \(m_1/m_2\) | 0.00030 |         |                       |            |
| sum (f1+f2) or (f3+f4) | 8.83878 |         | 8.83909               | 8.83894 ± 0.00016 avg. |
| f5 eVP correction (Uehling), \(\alpha(Z\alpha)^4\) | 0.00575 | 0.00575 | 0.0057361 39 Tab.IV | 0.0057361 K |
| f6 2nd order eVP corr. (KS), \(\alpha^2(Z\alpha)^4\) | 0.00005 | 0.00005 | 0.0000501 37 Tab.IX “eVP2” | 0.0000501 K |
| f7a \(\alpha(Z\alpha)^4m, \text{like #11}\) | 0.0000127 | 0.0000127 | Tab.IX (a) | 0.0000127 K |
| f7d \(\alpha(Z\alpha)^4m, \text{like #12}\) | 0.0000991 | 0.0000991 | Tab.IX (d) | 0.0000991 K |
| f7e \(\alpha^2(Z\alpha)^4m, \text{like #30*}\) | 0.00000012 | Tab.IX (e) | 0.0000012 K |
| f8 AMM (second order) | 0.01949 |         |                       |            |
| f9 AMM (higher orders) | 0.00007 |         |                       |            |
| sum Total AMM (f8+f9) | 0.01957 | 0.01956 | 0.019565 ± 0.000005 avg. |            |
| f10 Finite size | −0.00028 | −0.00027 | −0.000274 * |            |
| Sum | 8.86387 | 8.86419 | 8.86412 ± 0.00016 |            |

* This is item (r8), evaluated for the deuteron radius from Eq. (5), see text.

V. 2P FINE STRUCTURE

The contributions to the 2P\(_{3/2}\)-2P\(_{1/2}\) fine structure splitting in muonic deuterium are displayed in Tab. VI.

The main contributions to the fine structure have only been calculated by Borie 22 and Martynenko’s group 23 24. For the latter, we refer to the more recent paper Ref. 24. The values agree in both papers.

As always, Borie starts from the Dirac equation, which has to be corrected for recoil effects. This sum of entries (f1)+(f2) has to be compared to Martynenko’s leading term (f3), corrected for relativistic effects (f4) which are automatically included in the Dirac equation. The result of both approaches agree reasonably well and we adopt the average 8.83894 ± 0.00016 meV.

The relativistic recoil correction of order \(\alpha(Z\alpha)^4\), (f5), has been calculated including all recoil corrections of order \(m/M\) by Karshenboim 30. This value thus supersedes 39 the values obtained by Borie 22 and Martynenko 23 24.

The Källén-Sabry term, item (f6), agrees nicely among all authors. Karshenboim et al. have evaluated some higher order \(\alpha^2(Z\alpha)^4m\) contributions with great accuracy 37 which we list as (f7a), (f7d), and (f7e). These terms originate from the same graphs as the Lamb shift items #11, #12, and #30*, shown in Figs. 6 7 and 9 respectively.

Contributions from the anomalous magnetic moment of the muon in second (f8) and higher (f9) orders have been calculated by Borie and Martynenko et al., and their sums agree.

A finite size correction to the 2P\(_{1/2}\) state (f10) is included, too. This term is the same term as item (r8) of the \(r^2\)-dependent contributions to the Lamb shift, but with the opposite sign (see discussion in Sec. III.B). We evaluate (r8) for the deuteron radius from Eq. (5) and obtain for our choice of the item (f10) −0.0000606 \(r^2\) = −0.000274 ± 6 · 10\(^{-8}\) meV.

Summing up we obtain as our choice for the 2P\(_{3/2}\)-2P\(_{1/2}\) fine structure splitting in muonic deuterium

\[
\Delta E_{fs}(2P_{3/2} - 2P_{1/2}) = 8.86412(16) \text{ meV.} \tag{43}
\]

VI. 2P LEVELS

The various 2P levels displayed in Fig. 1 are separated by the 2P fine structure treated in Sec. V and further split by the 2P hyperfine splitting caused by the magnetic hyperfine interaction and the electric quadrupole interaction. The Breit-Pauli Hamiltonian can be displayed in...
matrix form as a sum of the magnetic HFS matrix and the quadrupole interaction matrix:

\[
M_{\text{Breit–Pauli}} = \begin{pmatrix}
-1.381777 & 0 & -0.126405 & 0 & 0 \\
0 & 0.690889 & 0 & -0.199864 & 0 \\
-0.126405 & 0 & 8.161148 & 0 & 0 \\
0 & -0.199864 & 0 & 8.582931 & 0 \\
0 & 0 & 0 & 0 & 9.285903
\end{pmatrix}_{\text{magnetic HFS}}
\]

\[
+ \begin{pmatrix}
0 & 0 & 0.613872 & 0 & 0 \\
0 & 0 & 0 & -0.194123 & 0 \\
0.613872 & 0 & 0.434073 & 0 & 0 \\
0 & -0.194123 & 0 & -0.347258 & 0 \\
0 & 0 & 0 & 0 & 0.086815
\end{pmatrix}_{\text{quadrupole int.}}
\]

(44)

It attains off-diagonal elements from mixing of levels with the same total angular momentum \( F \), but differ-
ent total muon angular momentum \( j \) [18, 22, 33, 81], as shown in Tab. VII. Note that the diagonal terms of the quadrupole interaction lead to a change in the order of the 2P\(_{3/2} \) levels (see also Fig. 1).

We follow Borie’s treatment [22], see also Pachucki [18] and Jentschura [30], but use our value for the 2P fine structure \( \Delta E_{2\pi}(2P_{3/2} - 2P_{1/2}) = 8.86412(16) \) meV from Sec. V Eq. (43), as well as a more recent value of the deuteron quadrupole moment

\[
Q = 0.285783(30) \text{ fm}^2
\]

(45)

from Ref. [82], or, equivalently, \( Q = 7.33945(77) \cdot 10^{-24} / \text{meV}^2 \), using \( \hbar c = 197.3269718(44) \text{ MeV fm} \) [4].

The numerical values of the quantities used in Tab. VII are given in Tab. VIII. In brief, \( \beta_D \) is defined in Eq. (22). For the 2P levels, \( \beta'_D = \beta_D(1 + \epsilon_2 \nu) \) (46) has to be used which contains the Uehling correction required for levels with \( \ell > 0 \) (see p. 25 and Eq. (12) in

| \( j \) | \( j' \) | magnetic HFS | Energy |
|---|---|---|---|
| 1/2 | 1/2 | \( (\beta_D'/6)(2 + x_a)\left[\delta_{F,1/2} + 1/2 \delta_{F,3/2}\right] \) | |
| 3/2 | 3/2 | \( \Delta E_{2\pi} + \left(\beta_D'/4\right)(4 + 5 x_a - a_p) \times \left[-1/6 \delta_{F,1/2} - 1/15 \delta_{F,3/2} + 1/10 \delta_{F,5/2}\right] \) | |
| 3/2 | 1/2 | \( \left(\beta_D'/48\right)(1 + 2 x_a - a_p)\left[-\sqrt{2} \delta_{F,1/2} - \sqrt{5} \delta_{F,3/2}\right] \) | |
| quadrupole interaction | | | |
| 1/2 | 1/2 | 0 | |
| 3/2 | 3/2 | \( \epsilon_Q \left[\delta_{F,1/2} - 4/5 \delta_{F,3/2} + 1/5 \delta_{F,5/2}\right] \) | |
| 3/2 | 1/2 | \( \epsilon_Q \left[\sqrt{2} \delta_{F,1/2} - 1/\sqrt{5} \delta_{F,3/2}\right] \) | |
TABLE VIII. Input parameters for the transition matrix. We recalculated Borie’s values, but use our fine structure (see Sec. V) and an updated value of the quadrupole moment Q recalculated from Borie’s values, but use our fine structure (see Eq. (48)).

| Parameter | Borie [22] | Our value |
|-----------|------------|-----------|
| $\beta_D$ | 4.0906 meV | 4.0906259 meV |
| $\beta_D'$ | 4.0922 meV | 4.092253 meV |
| $\epsilon_Q$ | 0.43439 meV | 0.43407(46) meV |
| $\alpha$ | 0.0248 | 0.0247889 |
| $a_\mu$ | 0.0011592 | |
| $\Delta E_{fs}$ | 8.86419 meV | 8.86412(16) meV |

Ref. [22]. For muonic deuterium,

$$\epsilon_{2P} = 0.000391. \quad (47)$$

The quadrupole moment of the deuteron enters in the hyperfine splitting via the quadrupole interaction, see Borie [22], pp. 24 and 25.

$$\epsilon_Q = \frac{\alpha Q (\alpha Z m_e)^3}{24} (1 + \epsilon_{2P}), \quad (48)$$

where Q the quadrupole moment of the deuteron and $\epsilon_{2P}$ is given in Eq. (47).

Diagonalizing the matrix Eq. (44) results in shifts of the 2P($F = 1/2$) and 2P($F = 3/2$) levels by

$$\Delta_{1/2} = 0.02376 \text{ meV} \quad \text{and} \quad \Delta_{3/2} = 0.02052 \text{ meV}, \quad (49)$$

respectively, as displayed in Fig. 1. The resulting energies of the various 2P sublevels are summarized in Tab. IX.

TABLE IX. 2P levels from fine- and hyperfine splitting. All values are in meV relative to the 2P$_{1/2}$ level. The fine structure ($2P_{3/2}$−2P$_{1/2}$ energy splitting) is our value $\Delta E_{fs} = 8.86412(16)$ meV from Eq. (43). Uncertainties arise from the quadrupole moment Q in Eq. (45) and $\Delta E_{fs}$.

| Level | Borie [22] | Our value |
|-------|------------|-----------|
| 2P$_{1/2}$ | $-1.4056$ | $-1.40554(1)$ |
| 2P$_{3/2}$ | $0.6703$ | $0.67037(1)$ |
| 2P$_{1/2}$ | $8.6194$ | $8.61898(17)$ |
| 2P$_{3/2}$ | $8.2560$ | $8.25619(16)$ |
| 2P$_{5/2}$ | $9.3728$ | $9.37272(16)$ |

VII. SUMMARY

In summary, we have compiled all known contributions to the Lamb shift, the 2P fine structure, and the 2S and 2P hyperfine splittings, from QED and nuclear structure contributions.

For the Lamb shift, the QED contributions in Tab. I show good agreement between the four (groups of) authors. A problem with our item #2 from Ref. [23] was identified and resolved by the authors. Ultimately, the uncertainty of these “pure QED” terms in Tab. I is sufficiently good.

For the radius-dependent terms in Tab. III we find good agreement between the authors, too. Some terms have however been calculated by only one group. We re-calculate a small term (r3') to verify that the model-dependence imposed by this contribution is sufficiently small.

The main limitation for the Lamb shift, and hence the deuteron charge radius to be extracted from the upcoming data, originates from the two-photon exchange contribution to the Lamb shift in $\mu d$. Here, a superficial inspection of the six modern values published in five papers since 2011 [55, 58, 60, 64, 65] vary between 1.68 meV and 2.01 meV, suggesting an uncertainty as large as 0.3 meV. The term-by-term comparison of the individual contributions in Tab. IV revealed that the agreement is in fact much better. Fruitful discussions with the authors of these papers and other experts in the field revealed missing terms and resulted in updated values of some individual terms. It is very reassuring that vastly different approaches give results in excellent agreement, when corrected for missing terms: zero-range approximation, modern nuclear models like AV18 (from two groups of authors) and $\chi$EFT-inspired NN-forces up to N3LO order, and dispersion relations using electron-deuteron scattering data. Our average, 1.709 ± 0.020 meV is a reliable prediction for the deuteron polarizability contribution to the Lamb shift in $\mu d$.

For the 2S-HFS, several nuclear structure contributions have so far only been calculated by one group [15]: These are items (h22a), (h22b), and (h27b) in Tab. V which are rather large, and their uncertainties dominate the theoretical uncertainty for the 2S-HFS. This uncertainty will prevent us from obtaining a meaningful value of the Zemach radius of the deuteron from the measurement of the 2S-HFS in $\mu d$. An improved calculation of these items is therefore desirable.
For the 2P fine- and hyperfine splittings we collect all terms from the various authors, recalculate the matrix elements of the Breit-Pauli Hamiltonian with updated values of the 2P fine structure and the deuteron quadrupole moment. Diagonalizing this matrix Eq. (44) we obtain the 2P level energies, and their uncertainties.

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Appendix A: The Darwin-Foldy term

The Darwin-Foldy term, which is part of the Barker-Glover corrections (our item #17 in Tab. 1) has historically been subject of different definitions.

Pachucki and Karshenboim [49] argue that the DF term originates from the Zitterbewegung of the nucleus and is hence absent for a spin-1 nucleus such as the deuteron (as well as for the spin-0 \(^4\)He nucleus).

Khriplovich, Milstein and Sen’kov [51] argue that the DF term must be made a part of the rms charge radius to be consistent with electron scattering. In this case, the DF term is not absent for spin-1 nuclei such as the deuteron.

Friar, Martorell and Sprung [50] have emphasized that the DF-term can be alternatively considered as part of a recoil correction of order \(1/M^2\), or as the energy shift due to a part of the mean-square radius of the nuclear charge distribution. They advocate the second choice but admit that the first choice has to be used for the proton because ”it is unfortunately far too late to change these conventions for the hydrogen atom”. They recommend, however, to not extend the hydrogen atom conventions to other nuclei.

Jentschura has discussed the situation in some breadth [52] and concluded that the DF term should indeed be considered a contribution to the atomic energy levels due to the nuclear Zitterbewegung, supporting the “atomic physics” convention of Ref. [49]. The DF term is hence absent for the deuteron.

This “atomic physics” convention, in which the DF term is not a part of the rms charge radius, but rather a recoil correction of order \((Z\alpha)^4m^3/M^2\) to the energy levels, is the convention used in CODATA-2010 [4], see Eq. (26) and (27) therein. It is also the convention used in the most recent measurement of the H-D isotope shift [13] which is the origin of the difference of the squared rms radii of the deuteron and the proton given in Eq. (4). Moreover, it is the convention used for the proton radius in muonic hydrogen [3].

Therefore, to be able to directly compare the numerical values of the proton and deuteron rms charge radii obtained in electronic and muonic atoms, one must follow the “atomic physics” convention [4, 13, 49, 52], which is what we do.

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