Lamb Shift in Light Muonic Atoms - Revisited

E. Borie
Karlsruhe Institute of Technology, Institut für Hochleistungsimpuls and Mikrowellentechnik (IHM), Hermann-von-Helmholtzplatz 1, D-76344 Eggenstein-Leopoldshafen, Germany

Abstract
In connection with recent and proposed experiments, and new theoretical results, my previous calculations of the Lamb shift in muonic hydrogen will be reviewed and compared with other work. In addition, numerical results for muonic deuterium and helium will be presented. Some previously neglected (but very small) effects are included.

Introduction
The energy levels of muonic atoms are very sensitive to effects of quantum electrodynamics (QED), nuclear structure, and recoil, since the muon is about 206 times heavier than the electron [1].

A recent measurement of the Lamb shift in muonic hydrogen [2] has stimulated great renewed interest in the energy levels of muonic atoms. A number of theoretical analyses of the Lamb shift (the 2p-2s transition) in light muonic atoms have been published [3, 4, 5, 6, 7, 8, 9, 10, 11, 12] before the experiment was performed. The present paper repeats the independent recalculation of some of the most important effects [6] for hydrogen and deuterium [13], including some previously neglected (but very small) effects and extends the numerical calculations to the case of muonic helium. Some recent results by other authors are also discussed.

In the numerical calculations the fundamental constants from the most recent CODATA compilation ([14]) are used (with the exception of the fine structure constant, which was revised more recently), i.e.: \( \alpha^{-1}, \hbar c, m_\mu, m_e, m_u = 137.0359991, 197.32696 \text{ MeV} \cdot \text{fm}, 105.658367 \text{ MeV}, 0.5109989 \text{ MeV}, 931.494030 \text{ MeV} \), respectively.

The changes in these constants compared with CODATA 2002 ([15]) are too small to make any relevant difference in the results, but the most recent values are used anyway.

Also, the following properties of the proton and deuteron were used: \( m_p = 938.27203 \text{ MeV} / c^2, \mu_p = 2.79285 \mu_N, \) and \( R_p = 0.875(7) \text{ fm} \) (from [15]); this agrees with a recent determination by the group at Jefferson Laboratory [16]. Other recent values have been reported, for example \( 0.8418(7) \text{ fm} \) and \( 0.877(8) \text{ fm} \) [17]. In some cases calculations were performed for several values of \( R_p \). In addition (see [14]) \( m_d = 1875.613 \text{ MeV} / c^2, \mu_d = 0.85744 \mu_N, R_d = 2.139(3) \text{ fm} \) (from [15]), or \( R_d = 2.130(3) \text{ fm} \) ([18]). For the helium isotopes \( m_\alpha = 3727.379 \text{ MeV} / c^2, R_\alpha = 1.676(8) \text{ fm} \) ([19]), or \( R_\alpha = 1.681(4) \text{ fm} \) ([20]); \( m_{\text{He}^3} = 2808.391 \text{ MeV} / c^2 \) and \( \mu_{\text{He}^3} = -2.1275 \mu_N \). An old measurement of \( R_{\text{He}^3} = 1.844 \text{ fm} \) [21] has been superseded by newer results which range from 1.959(34) fm [22] or 1.961 fm [23].
to 1.975(4) fm [24] (other results are cited in these papers). Here an average value of 1.966(10) fm will be used for an estimate, since there is still some uncertainty in the calculations used in the newer determinations. In some cases, older values for the proton and deuteron radii were used to make comparison with earlier results [6,13] easier.

The deuteron has spin 1 and thus has both magnetic and quadrupole moments. The quadrupole moment of the deuteron is taken to be \( Q = 0.2860(15) \text{ fm}^2 \) [25, 26, 27]. A newer result [28] is nearly the same, but more precise.

**Vacuum Polarization**

The most important QED effect for muonic atoms is the virtual production and annihilation of a single \( e^+e^- \) pair. It has as a consequence an effective interaction of order \( \alpha Z \alpha \) which is usually called the Uehling potential [29, 30]. This interaction describes the most important modification of Coulomb’s law. Numerically it is so important that it should not be treated using perturbation theory; instead the Uehling potential should be added to the nuclear electrostatic potential before solving the Dirac equation. However, a perturbative treatment is also useful in the case of very light atoms, such as hydrogen.

Unlike some other authors, we prefer to use relativistic (Dirac) wave functions to describe the muonic orbit. This is more exact, and as will be seen below, it makes a difference at least for the most important contributions. Relativistic recoil corrections to this treatment will be calculated according to the prescription given in [1]. The wave functions are given in the book of Akhiezer and Berestetskii [31] and will not be given here. In perturbation theory, the energy shift due to an effective potential \( \Delta V \) is given by

\[
\Delta E_{\text{nr}} = \frac{1}{2\pi^2} \int_0^\infty q^2 dq \Delta V(q) \cdot \int_0^\infty dr j_0(qr) [F_{nk}^2 + G_{nk}^2] 
\]

where \( F_{nk} \) and \( G_{nk} \) are the small and large components of the wave function, \( n \) is the principle quantum number and \( \kappa \) is equal to \( -\ell - 1 \) if \( j = \ell + \frac{1}{2} \) and \( +\ell \) if \( j = \ell - \frac{1}{2} \). \( \Delta V(q) \) is the Fourier transform of the physical potential.

\[
\Delta V(q) = 4\pi \cdot \int_0^\infty r^2 \cdot j_0(qr) \cdot \Delta V(r) \, dr 
\]

\[
\Delta V(r) = \frac{1}{2\pi^2} \cdot \int_0^\infty q^2 \cdot j_0(qr) \cdot \Delta V(q) \, dq 
\]

As is well-known [1], the Uehling potential in momentum space is given by

\[
V_{\text{Ueh}}(q) = -\frac{4\alpha(\alpha Z)}{3} \cdot G_E(q) \cdot F(\phi) = -4\pi(\alpha Z) \cdot G_E(q) \cdot U_2(q)
\]

where \( G_E \) is the proton charge form factor, \( \sinh(\phi) = q/(2m_e) \) and

\[
F(\phi) = \frac{1}{3} + (\coth^2(\phi) - 3) \cdot [1 - \phi \cdot \coth(\phi)]
\]

\( U_2(q) \) is also defined in [1]. If the correction to the transition \( 2p_{1/2} - 2s_{1/2} \) is calculated in lowest order perturbation theory using nonrelativistic point Coulomb wave functions, the result is 205.0074 meV, in agreement with other authors [3].
The same procedure was used to calculate the two-loop corrections; the corresponding diagrams were first calculated by Källen and Sabry [32]. The Fourier transform of the corresponding potential is given in [1, 7]. The result for a point nucleus is 1.5080 meV.

In momentum space including the effect of nuclear size on the Uehling potential is trivial, since the corresponding expression for $\Delta V(q)$ is simply multiplied by the form factor. The numbers obtained were the same for a dipole form factor and for a Gaussian form factor, provided the parameters were adjusted to reproduce the assumed rms radius of the proton. The correction can be regarded as taking into account the effect of finite nuclear size on the virtual electron-positron pair in the loop. The contribution of the Uehling potential to the 2p-2s transition is reduced by 0.0079 meV with a proton radius of 0.842 fm [2], and by 0.0082 meV with a proton radius of 0.875 fm [15]. This result is consistent with the number given in [3] (eq.(266)). The contribution due to the Källen-Sabry potential is reduced by 0.00007 meV.

These numbers are modified somewhat when relativistic (Dirac) muon wave functions are used. The numerical values given below were calculated as the expectation value of the Uehling potential using point-Coulomb Dirac wave functions with reduced mass:

| point nucleus                                      | $R_p=0.875\text{fm}$ |
|----------------------------------------------------|----------------------|
| Uehling                                            | $2p_{1/2} - 2s_{1/2}$ | $2p_{1/2} - 2s_{1/2}$ | $2p_{3/2} - 2s_{1/2}$ | $2p_{3/2} - 2s_{1/2}$ |
|                                                    | 205.0282             | 205.0332             | 205.0198             | 205.0248             |
| Kaellen-Sabry                                      | 1.50814              | 1.50818              | 1.50807              | 1.50811              |

The effect of finite proton size calculated here was checked for several values of the proton radius, ranging from 0.842 fm to 0.892 fm. It can be parametrized as -0.0110\langle r^2 \rangle. The contribution due to two and three iterations has been calculated by [4, 35] and [34], respectively, giving a total of 0.1507 meV. An additional higher iteration including finite size and vacuum polarization is given in ref. [4] (equations(66) and (67)) and ref. [3] (equations(264) and (268)). This amounts to -0.0164\langle r^2 \rangle, and is verified in Appendix B. This would mean that the finite-size contributions to vacuum polarization in muonic hydrogen can be parametrized as $-0.0110\langle r^2 \rangle - 0.0164\langle r^2 \rangle$, giving a total of $-0.0274\langle r^2 \rangle$. Numerically this is -0.0209(6) meV if the proton radius is 0.875 fm, or -0.0194 meV if the proton radius is 0.842 fm.

Up to now the higher order effect including nuclear size has only been calculated for hydrogen. The contribution for other light nuclei is given in Appendix B.

Corresponding numbers for muonic deuterium, calculated as the expectation value of the Uehling potential using point-Coulomb Dirac wave functions with reduced mass are:

| point nucleus                                      | $R_d=2.139\text{fm}$ |
|----------------------------------------------------|----------------------|
| Uehling                                            | $2p_{1/2} - 2s_{1/2}$ | $2p_{3/2} - 2s_{1/2}$ | $2p_{1/2} - 2s_{1/2}$ | $2p_{3/2} - 2s_{1/2}$ |
|                                                    | 227.6577             | 227.6635             | 227.5986             | 227.6043             |
| Kaellen-Sabry                                      | 1.66622              | 1.66626              | 1.66577              | 1.66581              |

The effect of finite nuclear size calculated here can be parametrized as $-0.0130\langle r^2 \rangle$. However higher iterations will change these results. The correction for a point nucleus has been calculated for muonic deuterium [35], giving an additional correction of 0.1718 meV. The effect of finite size as described in refs. [3, 4] is given in Appendix B and results in an additional contribution to the binding energy of the 2s-state of $-0.02062\langle r^2 \rangle$, or $-0.0936\text{meV}$ for a deuteron radius of 2.130 fm.
Corresponding numbers for muonic $^3$He and $^4$He, calculated as the expectation value of the Uehling potential using point-Coulomb Dirac wave functions with reduced mass are:

|        | point nucleus | $R_{He} \neq 0$ |
|--------|---------------|-----------------|
| $^4$He | $2p_{1/2} - 2s_{1/2}$ | $2p_{1/2} - 2s_{1/2}$ |
| Uehling| 1666.305      | 1665.381        |
|        | 1666.580      | 1665.656        |
| Kaellen-Sabry | 11.5731     | 11.5658         |
|        | 11.5752       | 11.5680         |
| $^3$He | $2p_{1/2} - 2s_{1/2}$ | $2p_{3/2} - 2s_{1/2}$ |
| Uehling| 1642.412      | 1641.337        |
|        | 1642.682      | 1641.607        |
| Kaellen-Sabry | 11.4107     | 11.4024         |
|        | 11.4128       | 11.4045         |

Here the nuclear radii were taken to be $R_{He^3}=1.966$ fm and $R_{He^4}=1.681$ fm. The effect of finite nuclear size calculated here (and with other radii) can be parametrized as $-0.3297\langle r^2 \rangle$ for $^4$He and $-0.3176\langle r^2 \rangle$ ($-0.3151\langle r^2 \rangle$ if the two-loop contribution is neglected) for $^3$He. Higher iterations change these results. In [1] they were calculated to be about 1.70 meV, including the effect of finite nuclear size, for $^4$He and 1.4 meV $^3$He. A more recent calculation of the correction for a point nucleus has been made for muonic $^4$He [35], giving a correction of 1.709 meV. The effect of finite nuclear size on the shift of the 2s-state is given in Appendix B (for both isotopes).

The mixed muon-electron vacuum polarization correction was recalculated and gave the same result as obtained previously, namely 0.00007 meV. [36, 3]. For deuterium, the contribution is 0.00008 meV, for $^3$He it is 0.00200 meV, and for $^4$He it is 0.00208 meV. For the helium isotopes, neglecting finite nuclear size would increase the contribution by 0.0001 meV.

The Wichmann-Kroll [33] contribution was calculated using the parametrization for the potential given in [1]. The result obtained for hydrogen is -0.00103 meV, consistent with that given in [3]. For deuterium, the contribution is -0.00111 meV. Values for both helium isotopes have also been calculated. The contribution is -0.01984 meV for $^4$He and -0.01969 meV for $^3$He. The reason for the negative sign is discussed in the review of Eides et al. [3].

The sixth order vacuum polarization corrections to the Lamb shift in muonic hydrogen have been calculated by Kinoshita and Nio [34]. Their result for the 2p-2s transition (in hydrogen) is

$$\Delta E^{(6)} \approx 0.00761 \text{ meV}$$

Recently Karshenboim et al. [35, 37] have recalculated all of the relevant graphs, and reproduced these results for hydrogen, including a correction that reduced the contribution to 0.00752 meV. In addition they performed a recalculation of the virtual Delbrück effect that is consistent with, but probably more accurate, than the results given in [38] and [1], possibly due to a more accurate numerical evaluation of the sevenfold integrals over Feynman parameters. The published results are given as the sum of this, the Wichmann-Kroll contribution and the previously uncalculated light by light contribution. In the case of muonic hydrogen and helium, the virtual Delbrück contribution very nearly cancels the Wichmann-Kroll contribution, so the total result can be expected to be small.
Numerically, they found the following total "light-by-light" corrections (i.e. the sum of the Wichmann-Kroll, virtual Delbrück and previously uncalculated term), in meV:

| Term                  | Value        |
|-----------------------|--------------|
| $\Delta E(\mu H)$    | -0.00089(2)  |
| $\Delta E(\mu D)$    | -0.00096(2)  |
| $\Delta E(\mu^4 He)$ | -0.00136(6)  |

The hadronic vacuum polarization contribution has been estimated by a number of authors [39, 40, 3]. It amounts to about 0.012 meV in hydrogen, 0.013 meV in deuterium, 0.219 meV in $^3$He and 0.225 meV in $^4$He. An uncertainty of about 5% should be expected.

**Finite nuclear size and nuclear polarization**

The main contribution due to finite nuclear size has been given analytically to order $(\alpha Z)^6$ by Friar [41]. The main result is:

$$\Delta E_{ns} = -\frac{2\alpha Z}{3} \left( \frac{\alpha Z m_r}{n} \right)^3 \cdot \left[ \langle r^2 \rangle - \frac{\alpha Z m_r}{2} \langle r^3 \rangle_{(2)} + (\alpha Z)^2 (F_{REL} + m_r^2 F_{NR}) \right] \quad (5)$$

Radiative corrections to the main term have been calculated by Eides and Grotch [42]. They contribute an additional correction of

$$\Delta E_{ns} = -\frac{2\alpha Z}{3} \left( \frac{\alpha Z m_r}{n} \right)^3 \cdot \alpha^2 Z (23/4 - 4 \ln(2) - 3/4) \cdot \langle r^2 \rangle$$

This correction (of order $\alpha (\alpha Z)^5$) amounts to an additional (fractional) correction to the main term equal to 2.2275 meV $r^2$ without the radiative correction; it is modified to -5.1973 meV $r^2$ with the correction. For muonic hydrogen, the main coefficient of $\langle r^2 \rangle$ is -5.1973 meV $r^2$ without the radiative correction; it is modified to -5.1979 meV $r^2$ with the correction. For the main term, the shift is -3.979 ± 0.076 meV if the proton rms radius is 0.875 ± 0.007 fm and -3.685 ± 0.008 meV if the proton rms radius is 0.842 ± 0.001 fm. The radiative correction increases these numbers by 0.0005 meV. Assuming a proton rms radius of 0.875 fm, the correction from the first two terms in Eq. (5) to the 2s-level is 3.956 meV for a dipole form factor and 3.958 meV for a Gaussian form factor. The parameters were fitted to the proton rms radius. The difference is due to the second term in Eq. (5). It contributes 0.009126 $\langle r^3 \rangle_{(2)}$ meV (or 0.0232 meV for a dipole form factor and 0.0212 meV for a Gaussian form factor).

Pachucki [5] has estimated a correction similar to the second term (proportional to $\langle r^3 \rangle_{(2)}$) in Eq. (5). Friar and Sick [43] have shown that the results are equivalent, at least for static potentials.
Since the second term in Eq.(5) is numerically important, it has been investigated further, at least for the case of hydrogen. The third Zemach moment was calculated in a model-independent manner from electron-proton scattering data by Friar and Sick [43], with the result $\langle r^3 \rangle_{(2)} = 2.71(13)\text{fm}^3$, for a contribution of 0.0247 meV, with an uncertainty of 0.0012 meV. and more recently, using new experimental results, by Distler et al. [44], with the result $\langle r^3 \rangle_{(2)} = 2.85(8)\text{fm}^3$, for a contribution of 0.0260 meV, with an uncertainty of 0.0007 meV. The relationship between the third Zemach moment and the charge radius will be discussed below.

Since the coefficient of $\langle r^2 \rangle$ is important for the determination of the nuclear radius, the terms of order $(\alpha Z)^6$ in Eq.(5) that depend only on this quantity are separated from the other terms. This affects only $(\alpha Z)^2 F_{\text{REL}}$. Details will be given in Appendix B. The result is an extra contribution to the energy shift of the 2s-state equal to

$$\Delta E_{2s} = \frac{2}{3} \frac{(\alpha Z)^6 m_r^3}{n^3} \langle r^2 \rangle [\gamma - \frac{35}{16} + \ln(\alpha Z)]$$

($\gamma$ is Euler’s constant). This results in an energy shift of $-0.00181\langle r^2 \rangle = -0.00138\text{meV}$ in hydrogen. The value of the coefficient is compatible with the estimated contribution of $-0.0016\langle r^2 \rangle$ given in ref. [2]. The other remaining terms (of order $(\alpha Z)^6$) given in [44] contribute 0.000123 meV if an exponential charge distribution is used. Some details are given in Appendix B. This estimate includes all of the terms in Eq.(5), while other authors [3, 5] give only some of them.

Friar [44] also found finite size contributions to the binding energy of the 2p-levels, amounting to

$$\Delta E_{np1/2} = \frac{(\alpha Z)^6 m_r}{3} \left( \frac{\alpha Z m_r}{n} \right)^3 \cdot \left( 1 - \frac{1}{n^2} \right) \left[ \frac{\langle r^2 \rangle}{2} + \frac{m_r^2 \langle r^4 \rangle}{15} \right]$$  \hspace{1cm} (6a)$$

$$\Delta E_{np3/2} = (\alpha Z) \left( \frac{\alpha Z m_r}{n} \right)^5 \cdot \frac{(n^2 - 1) \langle r^4 \rangle}{45}$$  \hspace{1cm} (6b)$$

If terms of order $(\alpha Z)^6$ are included in the coefficient of $\langle r^2 \rangle$ are to be taken into account consistently, the contribution to the 2p_{1/2} energy level must also be included. For hydrogen, this is $-0.0000519\langle r^2 \rangle = -4\times10^{-5}\text{meV}$. Subtracting this contribution from the order $(\alpha Z)^6$ shift of the 2s level results in a contribution to the 2s_{1/2}-2p_{1/2} transition of 0.00131 meV, in good agreement with previous estimates [3]. There is no contribution to the coefficient of $\langle r^2 \rangle$ for transitions to the 2p_{3/2} state. The fine structure is, of course, affected. The contribution to the 2p_{1/2} energy level of deuterium, gives a correction of $-0.0000606\langle r^2 \rangle = -2.8\times10^{-4}\text{meV}$.

The contribution to the energy of the 2p_{3/2} state is much smaller, and is proportional to $\langle r^4 \rangle$; the relation to the rms-radius of the nucleus is model dependent. Analytic expressions for $\langle r^4 \rangle$ in terms of $\langle r^2 \rangle$ can be derived from the table given in ref. [11]. For an exponential charge distribution, $\langle r^4 \rangle = 5(\langle r^2 \rangle)^2/2$ and for a Gaussian charge distribution $\langle r^4 \rangle = 5(\langle r^2 \rangle)^2/3$. For the helium isotopes these corrections are significant for both levels.

These contributions, with numerical values for the coefficients and energy shifts for deuterium and helium will be given in Appendix B.

For the extraction of a single radius parameter from experimental data, it is useful, and has become customary, to write the Lamb shift in the form

$$\Delta E_{LS} = A + B\langle r^2 \rangle + C(\langle r^2 \rangle)^{3/2}$$
It is straightforward to determine $B$. There are several contributions, and these will be given in Appendix B, with numerical values for all cases. However, the value of $C$ depends on a model for the charge distribution, since it depends on the ratio

$$f = \frac{\langle r^3 \rangle}{(\langle r^2 \rangle)^{3/2}}$$

For Gaussian and exponential charge distributions, $f$ can be calculated analytically [11], with the result $f = 32/(3\sqrt{3\pi}) = 3.4745$ for a Gaussian charge distribution, and $f = 105/(16\sqrt{3}) = 3.7889$ for an exponential charge distribution, which corresponds to a dipole form factor. The corresponding coefficients of $(\langle r^2 \rangle)^{3/2}$ (in units meV fm$^{-3}$) are, for hydrogen, 0.03458 (dipole form factor) and 0.03171 (Gaussian form factor).

When the third Zemach radius is determined from experiment, the value of $f$ must also be determined from the same experimental data. Using the results of Friar and Sick [43, 45] gives $f = 3.780(52)$, while the newest evaluation [44] gives $f = 4.18(13)$. The corresponding coefficients of $(\langle r^2 \rangle)^{3/2}$ are 0.03485(5) and 0.0383(12), respectively. In the newest CODATA compilation [14] a value of $f = 3.4(2)$ is given. This is almost certainly too small in view of the previous values discussed. An average value of the two model independent determinations corresponds to $f = 4.0(2)$ and would result in a coefficient of 0.0365(18) meV fm$^{-3}$. The uncertainty in the precise value of the coefficient will have consequences for the theoretical uncertainty in the value of the proton radius, evaluated as in the recent experiment [2]. The value of $A$ also has a theoretical uncertainty, which may have been slightly underestimated. (see the summary tables and Appendix C).

The recommended contribution due to the third Zemach moment (expressed in terms of $(\langle r^2 \rangle)^{3/2}$) for deuterium is $(0.0112 f = 0.0448(22))$: 0.0448(22) meV fm$^{-3}$. The uncertainty in the precise value of the coefficient will have consequences for the theoretical uncertainty in the value of the proton radius, evaluated as in the recent experiment [2]. The value of $A$ also has a theoretical uncertainty, which may have been slightly underestimated. (see the summary tables and Appendix C).

The contribution due to nuclear polarization (in hydrogen) has been calculated by Rosenfelder [46] to be $0.017 \pm 0.004$ meV, and by Pachucki [5] to be $0.012 \pm 0.002$ meV. Other calculations [47, 48] give intermediate values ($0.013$ meV and $0.016$ meV, respectively). A very recent calculation [49] gives a unified treatment of elastic and inelastic contributions. The total given there is very close to the total that would be obtained in this work if only the inelastic contribution (0.0127(5)) is included in the nuclear polarization correction, and the Zemach moment contribution is interpreted as the sum of the other two contributions given there. However, the estimated error in the polarizability correction has been enlarged to be comparable to the total uncertainty.

The contribution due to nuclear polarization in deuterium has been calculated by Leidemann and Rosenfelder [50] to be $1.50 \pm 0.025$ meV (see also [51]). A newer calculation [52] gives $1.680 \pm 0.016$ meV. The author also claims that some inelastic contributions to the polarizability cancel the contribution due to the Zemach moment.

An estimate of the nuclear polarization contribution for the helium isotopes is given in [1, 53]. It amounts to $3.1 \pm 0.6$ meV for $^4$He and $4.9 \pm 1.0$ meV for $^3$He.

**Relativistic Recoil**

As is well-known, the center-of-mass motion can be separated exactly from the relative motion only in the nonrelativistic limit. Relativistic corrections have been studied by
many authors, and will not be reviewed here. The relativistic recoil corrections summarized in [1] include the effect of finite nuclear size to leading order in \( m_\mu /m_N \) properly. In fact the effect calculated here is probably accurate to order \( \alpha Z m_\mu /m_N \).

Up to 2004 this method was not used to treat recoil corrections to vacuum polarization. The recoil correction to the energy shift due to the Uehling potential can be included explicitly, as a perturbation correction to point-Coulomb values, in a manner very similar to that described in [1] (and in [41]). This was first described in [6]; the result in the case of hydrogen for the total relativistic correction agrees very well with an independent calculation based on a generalized Breit equation [56]. The basic formulas and numerical results are given here. Details are given in Appendix A. To leading order in \( 1/m_N \), the energy levels including a shift beyond that due to using the reduced mass in the Dirac equation are given by

\[
E = E_r - \frac{B_0^2}{2m_N} + \frac{1}{2m_N} \langle h(r) + 2B_0 P_1(r) \rangle
\]

where \( E_r \) is the energy level calculated using the Dirac equation with reduced mass and \( B_0 \) is the unperturbed binding energy. Also

\[
h(r) = -P_1(r)(P_1(r) + \frac{1}{r}Q_2(r)) - \frac{1}{3r}Q_2(r)[P_1(r) + \frac{1}{r^3}Q_4(r)]
\]

Here

\[
P_1(r) = 4\pi \alpha Z \int_r^\infty r' \rho(r')dr' = -V(r) - rV'(r)
\]

\[
Q_2(r) = 4\pi \alpha Z \int_r^\infty r'^2 \rho(r')dr' = r^2 V'(r)
\]

\[
Q_4(r) = 4\pi \alpha Z \int_0^r r'^4 \rho(r')dr' = r^4 V'(r) - 2r^3 V(r) + 6 \int_0^r r'^2 V(r')dr'
\]

Details for the case of vacuum polarization are given in Appendix A and in Ref. [6].

To obtain the full relativistic and recoil corrections, one must add the difference between the expectation values of the Uehling potential calculated with relativistic and nonrelativistic wave functions, giving a total correction of 0.0169 meV for muonic hydrogen. This is in very good agreement with the correction of 0.0168 meV calculated by

|            | Main term | Correction | Total   |
|------------|-----------|------------|---------|
| hydrogen   | 0.0210    | -0.0041    | 0.0169  |
| deuterium  | 0.0229    | -0.00246   | 0.0204  |
| \(^3\)He   | 0.527     | -0.032     | 0.495   |
| \(^4\)He   | 0.534     | -0.0248    | 0.509   |

**Table 1:** Total relativistic corrections due to vacuum polarization to the Lamb shift in light muonic atoms (in meV). The main term is the difference between the vacuum polarization contribution calculated with relativistic and nonrelativistic wave functions. The correction is calculated here.
Veitia and Pachucki [56]. The treatment presented here has the advantage of treating the main contribution relativistically and applying a small correction that can be calculated using first order perturbation theory. The Källen-Sabry contribution to the main term was included. For hydrogen, this adds 0.0002 meV to the main term. The results for all cases are summarized in Table 1.

A recent paper by Jentschura [57] overlooks the fact that a correction due to relativistic recoil was included in previous work [6] and adds an additional “correction” of -0.0039 meV to the Lamb shift of muonic hydrogen in Eq. (3.3). This amounts to double counting this contribution, which is listed in Table 3 (and in ref [6]) as a “recoil correction to VP”.

This method is also used to calculate relativistic recoil corrections to the shift due to finite nuclear size when a model for the charge distribution is given. This was done by Friar [41]; The recoil correction is given by:

$$\Delta E_r = -\frac{(\alpha Z)^2}{m_N} \left(\frac{\alpha Z m_r}{n}\right)^3 \langle r(2) \rangle \delta \ell_0.$$

Numerically the contribution due to finite nuclear size to the recoil correction for the binding energy of the 2s-level is -0.013 meV in hydrogen, and -0.019 meV in deuterium. The factor $1/m_N$ is replaced by $1/(m_N + m_N)$, also consistent with the calculations presented in [41]. In the case of hydrogen, the contribution is approximately 0.004 meV smaller if a Gaussian charge distribution is used instead of an exponential charge distribution. With the exponential charge distribution, the value of the contribution ranges from 0.0131 meV to 0.0139 meV as the charge radius varies from 0.842 fm to 0.895 fm. A calculation with the value given by Distler et al. [41] is also in this range. This contribution is thus nearly constant for hydrogen. For muonic $^4$He the recoil contribution is -0.267 meV for a Gaussian charge distribution and an rms-radius of 1.681 fm. Varying the radius by ±0.02 fm changes the contribution by ±0.003 meV. For muonic $^3$He this recoil contribution is -0.404 meV for a Gaussian charge distribution and an rms-radius of 1.966 fm.

The review by Eides et al. [3] gives a better version of the two photon recoil (Eq. 136) than was available for the review by Borie and G. Rinker [1]. Evaluating this expression for muonic hydrogen gives a contribution of -0.04497 meV to the 2p-2s transition in hydrogen, -0.02656 meV in deuterium, -0.4330 meV in $^4$He, and -0.5581 meV in $^3$He.

Higher order radiative recoil corrections give additional contributions [3]. These correspond to (their) Table 9 and two additional terms in Table 8. Numerically, the contributions are -0.01003 for hydrogen, -0.00302 for deuterium, -0.04737 for $^4$He and -0.08102 for $^3$He.

An additional recoil correction for states with $\ell \neq 0$ has been given by [58] (see also [3]). It is

$$\Delta E_{n,\ell,j} = \frac{(\alpha Z)^4}{2n^3m_N^2} \left(1 - \delta \ell_0\right) \left(\frac{1}{j + 1/2} - \frac{1}{\ell + 1/2}\right)$$

(10)

Note that $1/(j + 1/2) - 1/(\ell + 1/2) = 1/(\kappa(2\ell + 1))$. When evaluated for the 2p-states of muonic hydrogen, one finds a contribution to the 2p-2s transition energy of 0.05748 meV for the $p_{1/2}$ state and -0.02873 meV for the $p_{3/2}$ state. For $^3$He the contribution is 0.12654 meV for the $p_{1/2}$ state and -0.06327 meV for the $p_{3/2}$ state. For integer spin nuclei, there is an additional shift of the 2s-state, amounting to $-\alpha Z(\alpha Z m_r/n)^3/(2m_N^2)$ [55]. Numerical values for the energy shift of the 2p$_{1/2}$ and 2p$_{3/2}$ states of deuterium...
are: 0.01681 meV and -0.00840 meV, respectively. The total contribution for the 2p\textsubscript{1/2}-2s transition is then 0.06724 meV; the fine structure is unaffected. Numerical values for \(^4\text{He}\) are 0.07379 meV for the 2p\textsubscript{1/2} state, -0.03690 meV for the 2p\textsubscript{3/2} state, and -0.22137 meV for the 2s state.

A final point about recoil corrections is that in the case of light muonic atoms, the mass ratio \(m_\mu/m_N\) is considerably larger than the usual perturbation expansion parameter \(\alpha Z\).

### Muon Lamb Shift

For the calculation of muon self-energy and vacuum polarization, the lowest order (one-loop approximation) contribution is well-known, at least in perturbation theory. For a point nucleus, and neglecting possible contributions due to vacuum polarization, so that \(\nabla^2 V = -4\pi\alpha Z\rho\) (\(\rho\) is the nuclear charge density) is approximated by a delta function, giving \(V = -\alpha Z/r\) and

\[
\langle \nabla^2 V \rangle = -4\pi\alpha Z|\psi_{ns}(0)|^2 \delta_{10} = -4Z\alpha \left(\frac{Z\alpha m_r}{n}\right)^3 \delta_{10}
\]

one finds a contribution of -0.66788 meV for the 2s\textsubscript{1/2} - 2p\textsubscript{1/2} transition and -0.65031 meV for the 2s\textsubscript{1/2} - 2p\textsubscript{3/2} transition. For deuterium, the corresponding contributions are given by -0.77462 meV for the 2s\textsubscript{1/2} - 2p\textsubscript{1/2} transition and -0.75512 meV for the 2s\textsubscript{1/2} - 2p\textsubscript{3/2} transition. These numbers include muon vacuum polarization (0.016844 meV for hydrogen, 0.019682 meV in deuterium, 0.33225 in \(^3\text{He}\), and 0.34132 in \(^4\text{He}\)), and an extra term of order \((Z\alpha)^5\) as given in [3] for the 2s-state:

\[
\Delta E_{2s} = \frac{\alpha(\alpha Z)^5 m_\mu}{4} \cdot \left(\frac{m_r}{m_\mu}\right)^3 \cdot \left(\frac{139}{64} + \frac{5}{96} - \ln(2)\right)
\]

which contributes -0.00443 meV for hydrogen and -0.00518 meV for deuterium. For the helium isotopes the contributions are -0.17490 meV in \(^3\text{He}\) and -0.17967 meV in \(^4\text{He}\). These results, and the higher order corrections [1, 36] are summarized in Table 2.

The higher order contributions can be written in the form

\[
\Delta E_{LS}^{4,6} = \frac{1}{m_\mu^2} \cdot \langle \nabla^2 V \rangle \left[m_\mu^2 F'_{1}(0) + \frac{a_\mu}{2} + \frac{a_\mu}{m_\mu m_r} \left(\frac{dV}{dr} \cdot \vec{L} \cdot \vec{\sigma}_\mu\right)\right]
\]

where \(F_2(0) = a_\mu\); the higher order contributions (fourth and sixth) can be taken from the well-known theory of the muon’s anomalous magnetic moment: \(F_2(0) = a_\mu = \alpha/2\pi + 0.7658(\alpha/\pi)^2 + 24.05(\alpha/\pi)^3\). The fourth order contribution to \(F'_1(0)\) is 0.46994(\(\alpha/\pi\))^2 + 2.21656(\(\alpha/\pi\))^2 = 2.68650(\(\alpha/\pi\))^2 [1, 36]. These expressions include the fourth order electron loops [54] which dominate the fourth order contribution. The contribution of the electron loops alone is -0.00168 meV for the 2s\textsubscript{1/2} - 2p\textsubscript{1/2} transition and -0.00159 meV for the 2s\textsubscript{1/2} - 2p\textsubscript{3/2} transition. Including the rest, which is the same as for the electron [1], gives -0.00160 meV and -0.00164 meV, respectively. Since it is no more difficult to include the complete contribution to \(F'_1(0)\) and \(F_2(0)\) in the analysis, there is no reason not to do so. An additional contribution due to including the Kållén-Sabry correction with muon loops effectively adds \(-(41/162)(\alpha/\pi)^2\) to \(F'_1(0)\) [3]. This has been included in the higher order corrections.
| Transition | $2p_{1/2} - 2s_{1/2}$ | $2p_{3/2} - 2s_{1/2}$ |
|------------|----------------------|----------------------|
| Hydrogen   | -0.667882            | -0.650313            |
| second order | -0.001714          | -0.001647          |
| Total      | -0.669596            | -0.651960            |
| Deuterium  | -0.774616            | -0.755125            |
| second order | -0.002001          | -0.001926          |
| Total      | -0.776617            | -0.757051            |
| $^3$He     | -10.827368           | -10.504167           |
| second order | -0.033749          | -0.032515          |
| Total      | -10.861117           | -10.536672           |
| $^4$He     | -11.105708           | -10.776650           |
| second order | -0.034663          | -0.033406          |
| Total      | -11.140370           | -10.810056           |

Table 2: Contributions to the muon Lamb shift ($E(2p_{1/2}) - E(2s_{1/2})$) in muonic hydrogen, deuterium, $^3$He, and $^4$He, in meV.

The numbers given in Table 2 were calculated assuming that $\nabla^2 V$ can be approximated by a delta function. However, the potential should be corrected for vacuum polarization due to electron loops, and, at least for s-states, for the effect of finite nuclear size. This has been done a long time ago ([9, 65, 66, 67]) for the hyperfine structure, but up to now not completely for the "muon Lamb shift". In addition, a correction as a result of distortion of the wave function of the 2s-state due to vacuum polarization, has recently been calculated by Ivanov et al. [68]. Numerically the results agree with previous calculations [6, 13] for the case of the hyperfine structure of the 2s-state (as given in Eq. 19), when the effect of finite nuclear size is neglected.

Pachucki [4] has estimated an additional contribution of -0.005 meV corresponding to a vacuum polarization insert in the external photon for hydrogen. It is not clear to what extent this contribution is described by corrections to $\langle \nabla^2 V \rangle$ as described in Appendix C. A more recent calculation by Jentschura [57] gives a different result for this contribution. An independent recalculation is desirable and this will be presented for a part of the contribution in Appendix C. The effect of finite nuclear size (analogous to the Bohr-Weisskopf effect known for the hyperfine structure) will also be estimated there.

The numerical value of the partial correction to the 2s-2p transition calculated there is of the order of 0.002 meV for hydrogen, which is too small to account for the discrepancy in the proton radius. It is not included in Table 2, since corrections to the Bethe sum...
have not been calculated. However, this introduces an uncertainty in the theoretical value. Also the corrections are larger for other light nuclei. The total corrections calculated in Appendix C should be considered as uncertainties in the theoretical value for the Lamb shift.

Summary of contributions

Using the fundamental constants from the CODATA 2006 compilation ([14]), except where noted, one finds the transition energies in meV in Table 3. Here the main vacuum polarization contributions are given for a point nucleus, using the Dirac equation with reduced mass. Relativistic recoil corrections are given separately. Some uncertainties have been increased from the values given by the authors, as discussed in the text.

| Contribution                              | Value (meV) | Uncertainty (meV) |
|-------------------------------------------|-------------|-------------------|
| Uehling                                   | 205.0282    |                   |
| Källen-Sabry                              | 1.5081      |                   |
| VP iterations [4,35]                      | 0.1507      |                   |
| sixth order [35]                          | 0.00752     |                   |
| Total ”LBL” [37]                          | -0.00089    | 0.00002           |
| mixed mu-e VP                             | 0.00007     |                   |
| hadronic VP                               | 0.011       | 0.001             |
| recoil [3] (eq136)                        | -0.04497    |                   |
| recoil, higher order [3]                  | -0.0100     |                   |
| recoil, finite size [11]                  | 0.013       | 0.001             |
| recoil correction to VP [11]              | -0.0041     |                   |
| additional recoil [58]                    | 0.0575      |                   |
| muon Lamb shift                           | -0.66788    |                   |
| second order                              |              |                   |
| higher orders                             | -0.00171    |                   |
| nuclear size ($R_p$=0.875 fm)             |              | 0.007 fm          |
| main correction $B \cdot \langle r^2 \rangle$ | -4.002      | 0.064             |
| Zemach moment [11]                        | 0.0244      | 0.002             |
| remaining order $(\alpha Z)^6$ [11]       | -0.0001     |                   |
| polarization                              | 0.0127      | 0.003             |
| correction to the $2p_{1/2}$ level         | 0.00004     |                   |

Table 3: Contributions to the muonic hydrogen Lamb shift. The proton radius is taken from [15].

In the case of the muon Lamb shift, the numbers in Table 3 are for the $2s_{1/2} - 2p_{1/2}$ transition.

As calculated in appendix B (see Table 14), the finite size corrections for hydrogen can be parametrized as $-5.22718\langle r^2 \rangle + 0.00913\langle r^3 \rangle$), where energies are in meV and radii in fm. The total coefficient of $\langle r^2 \rangle$ differs slightly from that given in ref. [2] (-5.2262meV fm$^{-2}$). The difference is due partly to a more precise determination of the coefficient of order $(\alpha Z)^6$ and partly to the inclusion of the radiative correction given by Eides and Grotch.
Also, the shift of the $2p_{1/2}$-state is included. The second term can be approximated by $0.0365(18)(\langle r^2 \rangle)^{3/2}$. This results in a total transition energy (without hyperfine interaction) of $206.0592(60) - 5.22718\langle r^2 \rangle + 0.0365(18)\langle r^2 \rangle^{3/2}$. If the proton radius is taken to be $0.842(1)$ fm, the (total) nuclear size correction becomes $-3.6855 \pm 0.010$ meV. With a radius of $0.875(7)$ fm, it is $-3.978 \pm 0.065$ meV.

A recent paper by Carroll et al. [59] calculates the Lamb shift in muonic hydrogen relativistically and nonperturbatively. This is very useful progress in removing the limitations of perturbation theory. For what is supposed to be the same calculated transition energy they obtain $206.0604 - 5.2794\langle r^2 \rangle + 0.0546\langle r^2 \rangle^{3/2}$. It would have been helpful if they had provided more details about how they obtain corrections due to two- and three-loop vacuum polarization contributions (Kaellen-Sabry, sixth order, and higher orders), muon selfenergy and muon vacuum polarization, hadron vacuum polarization, relativistic recoil, and nuclear polarization. Instead they simply used the values listed in the supplement to ref. [2]. Also, there are some problems with their calculation of the hyperfine splitting of the $2s$ state.

**Summary of contributions for muonic deuterium**

Muonic deuterium is in many ways similar to muonic hydrogen, but there are some differences. In addition to the different mass, the deuteron has spin 1 and both magnetic and quadrupole moments. For deuterium, one finds the transition energies in meV in Table 4. Also here the main vacuum polarization contributions are given for a point nucleus, using the Dirac equation with reduced mass.

As calculated in appendix B (see Table 14), the finite size corrections for the $2s$-$2p$ transition in muonic deuterium can be parametrized as $-6.10940\langle r^2 \rangle + 0.0112\langle r^3 \rangle_{(2)}$. Where energies are in meV and radii in fm. The second term can be approximated by $0.0448(22)(\langle r^2 \rangle)^{3/2}$. For more details, including the contribution for remaining order $(\alpha Z)^6$, see appendix B. The total transition energy (without hyperfine structure) calculated here is then

$$230.2972 \pm 0.04 - 6.10940\langle r^2 \rangle + 0.0448(22)(\langle r^2 \rangle)^{3/2} \text{meV}$$

A very recent calculation of the same transition energy by Krutov and Martynenko [60] gives similar results, with one significant difference. For the nuclear structure contributions of order $(Z\alpha)^5$ they use the value given by Pachucki [52], which supposedly includes nuclear polarization and the Zemach moment term. In this work, the more standard separation is used. The total calculated here is approximately $0.433(21)+1.50(3)=1.933(45)$ meV, to be compared with $1.680(16)$ meV. The difference amounts to $0.256(60)$ meV, which is not negligible. An independent calculation of these nuclear structure effects would be very desirable.
| Contribution | Value (meV) | Uncertainty (meV) |
|--------------|------------|------------------|
| Uehling      | 227.6577   |                  |
| Källen-Sabry | 1.6662     |                  |
| VP iterations [35] |       | 0.1718          |
| sixth order [35] |   | 0.00842 0.00007 |
| Total ”LBL” [37] | -0.00096 0.00002 |
| mixed mu-e VP | 0.00008    |                  |
| hadronic VP   | 0.013      | 0.001            |
| recoil [3] (eq136) | -0.02656 |                  |
| recoil, higher order [3] | -0.00302 |                  |
| recoil, finite size [41] | 0.019 | 0.003            |
| recoil correction to VP [1] | -0.00246 |                  |
| additional recoil [58] | 0.06724 |                  |
| muon Lamb shift |            |                  |
| second order  | -0.774616  |                  |
| higher orders | -0.002001  |                  |
| nuclear size ($R_d=2.130\text{fm}$ [18]) | 0.003 fm |                  |
| main correction $B \cdot \langle r^2 \rangle$ | -27.718 0.078 |
| Zemach moment [41] | 0.4329 | 0.021            |
| remaining order $(\alpha Z)^6$ [41] | 0.0034 |                  |
| polarization [50] | 1.50 | 0.03             |
| correction to the 2p$_{1/2}$ level | 0.00038 |                  |

**Table 4:** Contributions to the muonic deuterium Lamb shift. The deuteron radius is taken from [18].

**Summary of contributions for muonic helium**

For $^4\text{He}$ one finds the transition energies in meV in table 5. Also here the main vacuum polarization contributions are given for a point nucleus, using the Dirac equation with reduced mass. In the case of $^4\text{He}$ results for two different radii (from [19, 20]) are given.
| Contribution                        | Value (meV) | Uncertainty (meV) |
|------------------------------------|-------------|-------------------|
| Uehling                            | 1665.388    |                   |
| Källen-Sabry                       | 11.566      |                   |
| VP iterations [35]                 | 1.709       |                   |
| sixth order [35]                   | 0.074       | 0.003             |
| Total ”LBL” [37]                   | -0.00136    | 0.00006           |
| mixed mu-e VP                      | 0.0021      |                   |
| hadronic VP                        | 0.228       | 0.012             |
| recoil [3] (eq136)                 | -0.4330     |                   |
| recoil, higher order [3]           | -0.0474     |                   |
| recoil, finite size [41]           | 0.2662      | 0.001             |
| recoil correction to VP [1]        | -0.0248     |                   |
| additional recoil [58]             | 0.2952      |                   |
| muon Lamb shift                    |             |                   |
| second order                       | -11.1057    |                   |
| higher orders                      | -0.0347     |                   |
| nuclear size ($R_{He}=1.676$ fm)  |             | 0.008 fm          |
| main correction $B \cdot \langle r^2 \rangle$ | -298.706 | 2.8               |
| Zemach moment [41]                 | 6.591       | 0.188             |
| remaining order ($\alpha Z)^6$ [41]| 0.055       |                   |
| correction to the $2p_{1/2}$ level | 0.0148      |                   |
| nuclear size ($R_{He}=1.681$ fm)  |             | 0.004 fm          |
| main correction $B \cdot \langle r^2 \rangle$ | -300.491 | 1.4               |
| Zemach moment [41]                 | 6.650       | 0.190             |
| remaining order ($\alpha Z)^6$ [41]| 0.057       |                   |
| correction to the $2p_{1/2}$ level | 0.0149      |                   |
| polarization [1, 53]               | 3.1         | 0.6               |

**Table 5:** Contributions to the muonic helium Lamb shift. Finite size contributions are given for two values of the nuclear radius of $^4$He.

As given in Table 14 in Appendix B, the finite size corrections for $^4$He can be parametrized as $-106.340\langle r^2 \rangle + 0.400\langle r^3 \rangle_{(2)}$, where energies are in meV and radii in fm. The second term can be approximated by $1.40(4)\langle r^2 \rangle^{3/2}$. The total transition energy would then be $1667.937 \pm 0.005 + 3.1 \pm 0.6 - 300.477 \pm 1.4 + 6.650 \pm 0.19 = 1377.210 \pm 1.5$ meV.

In previous work [1, 8], recoil corrections to the Lamb shift in $^4$He denoted by "two photon" and "Breit" were given as $-0.44$ meV and +0.28 meV, respectively. These clearly correspond to corrections given here as (recoil [3] (eq136)) of $-0.433$ meV and (recoil, finite size [41]) of $-0.1221$ fm$^{-1}\langle r \rangle_{(2)} = 0.266$ meV, respectively.

For $^3$He one finds the transition energies in meV in Table 6. Also here the main vacuum polarization contributions are given for a point nucleus, using the Dirac equation with reduced mass. From Table 14 in Appendix B, the finite size corrections for $^3$He can be parametrized as $-103.508(5)\langle r^2 \rangle + 0.3860\langle r^3 \rangle_{(2)}$, where energies are in meV and radii in fm. The second term can be approximated by $1.35(4)\langle r^2 \rangle^{3/2}$. This gives a total value of $1648.402 \pm 1.3 - 400.075 \pm 3.67 + 0.015 + 10.258 \pm 0.305 = 1258.600 \pm 1.5$ meV.
| Contribution                | Value (meV)   | Uncertainty (meV) |
|----------------------------|---------------|-------------------|
| Uehling                    | 1641.337      |                   |
| Källen-Sabry               | 11.402        |                   |
| VP iterations [1]          | 1.4           |                   |
| Wichmann-Kroll             | -0.0197       |                   |
| virt. Delbrueck [1]        | 0.02          |                   |
| mixed mu-e VP              | 0.0020        |                   |
| hadronic VP                | 0.221         | 0.011             |
| recoil [3] (eq136)         | -0.55811      |                   |
| recoil, higher order [3]   | -0.0810       |                   |
| recoil, finite size [41]   | 0.4040        | 0.0010            |
| recoil correction to VP [1]| -0.03196      |                   |
| additional recoil [58]     | 0.12654       |                   |

Table 6: Contributions to the muonic helium Lamb shift. The nuclear radius of $^3$He is taken to be 1.966(10) fm.

Here the estimated uncertainty does not include the uncertainty in the radius, but only the uncertainty in the coefficient of the Zemach moment and the nuclear polarization. This agrees quite well with a previous calculation [10], which was considerably less precise, when the change in the contribution due the more recent measured radius is taken into account.

**Fine structure of the 2p state**

The fine structure of the 2p states can be calculated by using the relativistic Dirac energies, computing the vacuum polarization contributions with Dirac wave functions, and including the effect of the anomalous magnetic moment in the muon Lamb shift. An additional recoil correction (Eq[10]) also has to be included. The results are summarized in Table 7. One should also include the $B^2/2M_N$-type correction to the fine structure. (see [3], Eq(38)). This is tiny ($5.7 \cdot 10^{-6}$ meV for hydrogen) and is not included in the table. As mentioned before, Friar [41] has given expressions for the energy shifts of the 2p-states due to finite nuclear size. A correction proportional to $\langle r^2 \rangle$ affects only the $2p_{1/2}$ state, and thus contributes to the fine structure. The contribution to the fine structure of the 2p-state of hydrogen ($4 \cdot 10^{-5}$ meV) is negligible. However, this contribution is not negligible for the helium isotopes. For hydrogen, this result for the fine structure was subsequently reproduced by Martynenko [61]. His results for the hyperfine structure of
Hydrogen deuterium $^3$He $^4$He

|                  | Hydrogen | deuterium | $^3$He | $^4$He |
|------------------|----------|-----------|--------|--------|
| Dirac            | 8.41564  | 8.86430   | 144.416| 145.718|
| Uehling (VP)     | 0.0050   | 0.00575   | 0.270  | 0.275  |
| Källen-Sabry     | 0.00004  | 0.00005   | 0.002  | 0.002  |

anomalous moment $a_\mu$

second order       | 0.01757  | 0.01949   | 0.3232 | 0.3290 |
higher orders      | 0.00007  | 0.00007   | 0.0012 | 0.0013 |
Recoil (Eq. 11)    | -0.08621 | -0.02521  | -0.1898| -0.1107|
Finite size        | -0.00004 | -0.00027  | -0.0158| -0.0119|
Total Fine Structure| 8.3521   | 8.86419   | 144.809| 146.203|

Table 7: Contributions to the fine structure ($E(2p_{3/2}) - E(2p_{1/2})$) of the 2p-state in muonic hydrogen, deuterium, $^3$He and $^4$He, in meV.

the 2p levels in hydrogen also agree with the results given below (and previously [6]). For deuterium, the fine structure agrees with that given by Krutov and Martynenko [60].

Hyperfine Interactions

The Breit equation [3, 9, 58] contributions to the fine- and hyperfine interactions for general potentials and arbitrary spins were given by Metzner and Pilkuhn [62]. Here a version applicable to the case of muonic atoms ($Z_1 = -1$, $s_1 = 1/2$, $m_1 = m_\mu$, $\kappa_1 = a_\mu$, $Z_2 = Z$) is given. For most of the following, the potential is approximated by $V_{\text{Coul}} = -\alpha Z/r$.

$$V_{L,s_1} = \frac{1}{2m_\mu} \frac{1}{r} \frac{dV}{dr} \left[ 1 + a_\mu - \frac{1}{m_\mu} \right] \vec{L} \cdot \vec{s}_1$$

(11)

This can be rearranged to give the well-known form for spin 1/2 nuclei with an anomalous magnetic moment, namely

$$-\frac{1}{r} \frac{dV}{dr} \cdot \frac{1 + a_\mu + (a_\mu + 1/2)m_N/m_\mu}{m_N m_\mu} \vec{L} \cdot \vec{a}_\mu$$

Note that

$$\frac{1}{m_N m_\mu} + \frac{1}{2m_\mu^2} = \frac{1}{2m_\mu^2} - \frac{1}{2m_N^2}$$

so that the terms not involving $a_\mu$ in the spin-orbit contribution are really the Dirac fine structure plus the Barker-Glover correction (Eq. 10).

Also

$$V_{L,s_2} = \frac{1}{2m_2} \frac{1}{r} \frac{dV}{dr} \left[ 1 + \kappa_2 - \frac{1}{m_2} \right] \vec{L} \cdot \vec{s}_2$$

Usually one writes

$$\frac{Z(1 + \kappa_2)}{m_2} = \frac{\mu_2}{m_\mu}$$

where $\mu_2$ is the magnetic moment of the nucleus in units of nuclear magnetons ($\mu_N = e/2m_p$). A value of $\mu_d = 0.85744 \mu_N = 0.307012 \mu_p$ corresponds to $\kappa_d = 0.714$. In the case of $^3$He, the magnetic moment is $\mu_{^3\text{He}} = -2.1275 \mu_N$, resulting in $\kappa_{^3\text{He}} = -4.184$.
The spin-spin interaction is given by

\[ V_{s_1s_2} = \frac{2(1 + a_\mu)\mu_2}{2s_2m_pm_m} \left[ \frac{1}{r} \frac{dV}{dr} \right] (3\hat{s}_1 \cdot \hat{r} \hat{s}_2 \cdot \hat{r} - \hat{s}_1 \cdot \hat{s}_2) - \frac{2}{3} \nabla^2 V \hat{s}_1 \cdot \hat{s}_2 \]

For deuterium the quadrupole moment also contributes, with

\[ V_Q = -\frac{Q}{2} \frac{1}{r} \frac{dV}{dr} \left[ 3\hat{s}_2 \cdot \hat{r} \hat{s}_2 \cdot \hat{r} - \hat{s}_2 \cdot \hat{s}_2 \right] \]

with \( Q \) in units of \( 1/m^2 \). The quadrupole moment of the deuteron is taken to be \( Q = 0.2860(15) \text{ fm}^2 \) \([25, 26, 27]\). In other units, one finds \( Q = 25.84/m^2 = 7.345 \times 10^{-6} \text{ MeV}^{-2} \).

The correction due to vacuum polarization (Eq. (13)) should be applied to the HFS shifts of the 2p-states, (and also to all spin-orbit terms in the "muon Lamb shift").

Note that for the 2p state

\[ \frac{1}{r} \frac{dV}{dr} \right|_{2p} \rightarrow \frac{1}{r} \frac{dV}{dr} \right|_{2p} \cdot (1 + \varepsilon_{2p}) \]

where

\[ \varepsilon_{2p} = \frac{2\alpha}{3\pi} \int_1^{\infty} \frac{(z^2 - 1)^{1/2}}{z^2} \cdot \left(1 + \frac{1}{2z^2}\right) \cdot \left(\frac{1}{(1 + az)^2} + \frac{2az}{(1 + az)^3}\right) dz \]

with \( a = 2m_e/(\alpha Zm_r) \). For hydrogen, \( \varepsilon_{2p} = 0.000365 \), for deuterium \( \varepsilon_{2p} = 0.000391 \) and for \(^3\text{He} \varepsilon_{2p} = 0.000894 \).

The correction due to vacuum polarization (Eq. (13)) should be applied to the HFS shifts of the 2p-states, (and also to all spin-orbit terms in the "muon Lamb shift").

Note that for the 2p state

\[ \frac{1}{r} \frac{dV}{dr} \right|_{2p} = \frac{2\alpha Z}{\ell(\ell + 1)(2\ell + 1)} \frac{(\alpha Zm_r/n)^3}{(\alpha Zm_r)^3} = \frac{\alpha Z(\alpha Zm_r)^3}{24} \]

The hyperfine structure can also be calculated relativistically, using the formalism given in \([1]\). The finite extent of the magnetization density and the effect of vacuum polarization should be taken into account also in this approach.

**Hyperfine structure of the 2s-state:**

The expectation value of \( V_{s_1s_2} \) in an \( n\)-s state with \( j = 1/2 \) is

\[ \Delta E_{ns} = 2\mu_2\alpha(\alpha Z)^3m^2 \frac{1}{3n^3m_pm_m} \cdot (1 + a_\mu)[F(F + 1) - s_2(s_2 + 1) - 3/4] \]

When \( s_2 = 1/2 \), and \( \mu_2/m_p = (1 + \kappa_2)/m_2 \), this reproduces the well-known result for muonic hydrogen (see, for example \([3]\), Eq. (271,277)):

\[ \Delta E_{ns} = 2\frac{\beta}{3m_pm_m} \cdot (1 + \kappa_2) \cdot (1 + a_\mu)(\nabla^2 V)[F(F + 1) - 3/2] = \frac{\beta}{2} (1 + a_\mu)[F(F + 1) - 3/2] \]
with
\[ \beta = \frac{8(\alpha Z)^4 m_r^3}{3n^3 m_p m_2} \cdot (1 + \kappa_2) = (8/n^3) \times 22.8054 \text{ meV} \] (14)

The numerical value was calculated for hydrogen. Note that \( \beta \cdot (1 + a_\mu) = 22.8320 \text{ meV} \), which is the well-known value. Since \(^3\text{He}\) also has spin 1/2, the same formula is valid, and one obtains \( \beta = -171.3964 \text{ meV} \). (\( \beta \cdot (1 + a_\mu) = -171.5963 \text{ meV} \))

For deuterium, with \( s_2 = 1 \), the corresponding hyperfine splitting is
\[ \Delta E_{ns} = \frac{2(\alpha Z)^4 m_r^3}{3n^3 m_p m_D} \cdot (1 + \kappa_D) \cdot (1 + a_\mu) \cdot [F(F + 1) - 11/4] \]
\[ = \frac{\beta_D}{2} \cdot (1 + a_\mu) \cdot [F(F + 1) - 11/4] = (8/n^3) \cdot 2.04766 \text{ meV} \cdot [\delta_{F3/2} - 2\delta_{F1/2}] \]
for a total splitting of 6.14298 meV in muonic deuterium. This is in reasonably good agreement with the result given by Carboni [12].

The QED corrections to the energy shift of the 2s-state were discussed in [3, 9]. In muonic hydrogen they are given by:
\[ \Delta E_{2s} = \beta \cdot (1 + a_\mu) \cdot (1 + \varepsilon_{VP} + \varepsilon_{\text{vertex}} + \varepsilon_{\text{Breit}} + \varepsilon_{\text{Zem}}) \cdot [\delta_{F1} - 3\delta_{F0}] / 4 \] (15)

The corrections due to QED effects, nuclear size and recoil are analogous for muonic deuterium and \(^3\text{He}\). Other corrections due to recoil, nuclear polarization, the weak interaction and so on can be included by adding corresponding \( \varepsilon \)'s. Here (3, Eq. (277))
\[ \varepsilon_{\text{Breit}} = \frac{17(\alpha Z)^2}{8} = 1.13 \cdot 10^{-4} \cdot Z^2 \]
is a relativistic correction that gives the difference between the value obtained in relativistic perturbation theory using Dirac wave functions, and the nonrelativistic value (to leading order in \( (\alpha Z)^2 \)). The vertex correction [3, 65] is given by
\[ \varepsilon_{\text{vertex}} = \alpha(Z\alpha) \left( \ln(2) - \frac{5}{2} \right) = -0.9622 \cdot 10^{-4} \cdot Z \]
This includes a correction of \( 3\alpha(Z\alpha)/4 = 0.3994 \cdot 10^{-4} \cdot Z \) due to muon loop vacuum polarization. Corrections due to hadronic vacuum polarization can be expected to be comparable to this value. Some higher order corrections to \( \varepsilon_{\text{vertex}} \) of order \( \alpha(Z\alpha)^2 \ln^2(Z\alpha) \) are possibly numerically important and were given in Ref. [65] as
\[ \frac{\alpha(Z\alpha)^2}{\pi} \left( -\frac{2}{3} \ln^2((Z\alpha)^{-2}) + c_{22}(2) \ln((Z\alpha)^{-2}) \right) = -0.0073 \cdot 10^{-4} \quad (Z = 1) \]
This correction adds an additional -0.00017 meV to the hyperfine splitting in the case of hydrogen (and -0.00004 meV in muonic deuterium). If \( Z = 2 \), the numerical value of the extra correction is \(-0.211 \times 10^{-4} \) and the contribution to the hyperfine splitting in muonic \(^3\text{He}\) is 0.0036 meV.
The main vacuum polarization correction has two contributions. One of these is a result of a modification of the magnetic interaction between the muon and the nucleus and is given by (see [10])

\[
\varepsilon_{VP1} = \frac{4\alpha}{3\pi^2} \int_0^\infty r^2 \, dr \left( \frac{R_{ns}(r)}{R_{ns}(0)} \right)^2 \int_0^\infty q^4 j_0(qr)G_M(q) \, dq \\
\int_1^\infty \frac{(z^2 - 1)^{1/2}}{z^2} \cdot \left( 1 + \frac{1}{2z^2} \right) \cdot \frac{dz}{4m_e^2[z^2 + (q/2m_e)^2]} \tag{16}
\]

One can do two of the integrals analytically and obtains for the 2s-state (with \( a = 2m_e/(\alpha Zm_r) \) and \( \sinh(\phi) = q/(2m_e) = K/a \))

\[
\varepsilon_{VP1} = \frac{4\alpha}{3\pi^2} \int_0^\infty \frac{K^2}{(1 + K^2)^2} F(\phi)G_M(\alpha Zm_rK) \, dK \left[ 2 - \frac{7}{(1 + K^2)} + \frac{6}{(1 + K^2)^2} \right] \tag{17}
\]

where \( F(\phi) \) is known from the Fourier transform of the Uehling potential and is given by Eq. (14).

The other contribution, as discussed by [65, 66] arises from the fact that the lower energy hyperfine state, being more tightly bound, has a higher probability of being in a region where vacuum polarization is large. This results in an additional energy shift of

\[
2 \int V_{Uehl}(r)\psi_{2s}(r)\delta_M\psi_{2s}(r)d^3r
\]

Following Ref. [65] with \( y = (\alpha Zm_r/2) \cdot r \), one has

\[
\delta_M\psi_{2s}(r) = 2\alpha Zm^2\Delta\nu_F\psi_{2s}(0) \left( \frac{2}{\alpha Zm_r} \right)^3 e^{-y} \left[ (1 - y)(\ln(2y) + \gamma) + \frac{13y - 3 - 2y^2}{4} - \frac{1}{4y} \right] \tag{18}
\]

(\( \gamma \) is Euler’s constant), and

\[
\psi_{2s}(r) = \psi_{2s}(0)(1 - y)e^{-y}
\]

One finds after a lengthy integration

\[
\varepsilon_{VP2} = \frac{16\alpha}{3\pi^2} \int_0^\infty \frac{dK}{1 + K^2}G_E(\alpha Zm_rK)F(\phi) \left\{ \frac{1}{2} - \frac{17}{(1 + K^2)^2} + \frac{41}{(1 + K^2)^3} - \frac{24}{(1 + K^2)^4} + \ln(1 + K^2) \left[ \frac{2}{1 + K^2} - \frac{7}{(1 + K^2)^2} + \frac{6}{(1 + K^2)^3} \right] + \frac{\tan^{-1}(K)}{K} \left[ \frac{19}{2(1 + K^2)} + \frac{20}{(1 + K^2)^2} - \frac{12}{(1 + K^2)^3} \right] \right\} \tag{19}
\]

Sternheim[66] denotes the two contributions by \( \delta_M \) and \( \delta_E \), respectively. An alternative expression, obtained by assuming a point nucleus, using Eq. (131) from [11] for the Uehling
potential, and doing the integrations in a different order, is

\[
\varepsilon_{VP2} = \frac{16\alpha}{3\pi} \int_{1}^{\infty} \frac{(z^2 - 1)^{1/2}}{z^2} \cdot \left(1 + \frac{1}{2z^2}\right) \cdot \frac{1}{(1 + az)^2} \cdot \left[\frac{az}{2} - \frac{1}{1 + az} + \frac{23}{8(1 + az)^2} - \frac{3}{2(1 + az)^3} + \ln(1 + az) \cdot \left(1 - \frac{2}{1 + az} + \frac{3}{2(1 + az)^2}\right)\right] dz
\]

with \(a = 2m_e/(\alpha Z m_{\text{red}})\) as in the case of \(\varepsilon_{2p}\). Both methods give the same result when the effect of nuclear size is neglected. In the case of ordinary hydrogen, each of these contributes \(3\alpha^2/8 = 1.997 \cdot 10^{-5}\). The accuracy of the numerical integration was checked by reproducing these results. One can thus expect that muonic vacuum polarization will contribute \(3\alpha^2/4 \simeq 4 \cdot 10^{-5}\), as in the case of normal hydrogen. This correction was included in \(\varepsilon_{\text{vertex}}\). Martynenko [70] includes only one of these contributions. The energy shift is approximately 0.00091 meV in hydrogen. Contributions due hadronic vacuum polarization should be slightly smaller. An estimate following the prescription given in [39] gives a correction of approximately \(0.2667 \cdot 10^{-4} \cdot Z\), or approximately 0.0006(1) meV in hydrogen. Contributions due to the weak interaction were estimated by Eides [75] and give \(5.8 \cdot 10^{-8}(m_\mu/m_e)E_F\), which works out to 0.00027 meV for the weak interaction contribution in muonic hydrogen. Unfortunately this calculation does not seem to be directly applicable to other nuclei.

Finite nuclear size has an effect on the value of \(\varepsilon_{VP}\). For muonic hydrogen, one obtains \(\varepsilon_{VP1} = 0.00211\) and \(\varepsilon_{VP2} = 0.00326\) for a point nucleus and \(\varepsilon_{VP1} = 0.00206\) and \(\varepsilon_{VP2} = 0.00321\) with a proton (magnetic) radius of 0.875 fm. Including this effect reduces the total contribution due to vacuum polarization by 0.00023 meV.

For muonic \(^3\)He, one obtains \(\varepsilon_{VP1} = 0.00295\) and \(\varepsilon_{VP2} = 0.00486\) including the effect of finite nuclear size. For a point nucleus the values would be \(\varepsilon_{VP1} = 0.00315\) and \(\varepsilon_{VP2} = 0.00506\).

For the case of muonic deuterium, \(\varepsilon_{VP1} = 0.00218\) and \(\varepsilon_{VP2} = 0.00337\) for a point nucleus. Including the effect of finite nuclear size gives \(\varepsilon_{VP1} = 0.00207\) and \(\varepsilon_{VP2} = 0.00326\).

The contribution to the hyperfine splitting of the 2s-state of muonic hydrogen (with finite extension of the magnetization density) is 0.04703 meV + 0.07328 meV = 0.12031 meV. The combined Breit and vertex corrections change this value to 0.11794 meV.

The contribution to the hyperfine structure from the two loop diagrams [32] can be calculated by replacing \(U_2(\alpha Z m_r, K) = (\alpha/3\pi)F(\phi)\) by \(U_4(\alpha Z m_r, K)\) (as given in [11 19]) in equations [17] and [19]. The resulting contributions in hydrogen are \(1.636 \cdot 10^{-5}\) and \(2.460 \cdot 10^{-5}\), respectively, giving a total shift of 0.00093 meV. Martynenko [70] neglected the contribution corresponding to Eq. [19]. The contributions in muonic deuterium are \(1.688 \cdot 10^{-5}\) and \(2.545 \cdot 10^{-5}\), respectively. For muonic \(^3\)He they are \(2.511 \cdot 10^{-5}\) and \(3.928 \cdot 10^{-5}\), respectively.

The correction due to \(\varepsilon_{VP2}\) can be regarded as a result of distortion of the wave function of the 2s-state, and has recently been calculated by Ivanov et al. [68]. Numerically their results agree with those given here to within a few one per cent, for both the second order and fourth order contributions in hydrogen and in deuterium. A more complete calculation of the vacuum polarization corrections to the 2s-state in hydrogen by the same authors [69] gives the same result for all these corrections to three significant figures, when nuclear
size is neglected. This paper includes the contribution of three further graphs, which give an additional contribution to $\epsilon_{VP_{tot}}$ of $1.64 \cdot 10^{-5}$, and a total two-loop contribution of 0.00130 meV to the hyperfine splitting of the 2s-state of hydrogen.

The main correction due to finite extension of the magnetization density is known as the Bohr-Weisskopf effect (67) and is equal to

$$\epsilon_{Zem} = -2\alpha Z m_r \langle r \rangle_{(2)}$$

where $\langle r \rangle_{(2)}$ is given in [9, 11, 43].

Ref. [4] claims that this correction does not treat off-shell effects and/or recoil properly. For hydrogen, Carlson et al. [73] give a recoil correction corresponding to $\epsilon_{rec} = 0.00093$, resulting in a correction of 0.02123 meV.

For hydrogen the value of $2\alpha Z m_r$ is $0.007024 \text{fm}^{-1}$. Using the value $\langle r \rangle_{(2)} = 1.086 \pm 0.012 \text{fm}$ from [43], gives a Zemach correction of $\epsilon_{Zem} = -0.00762$, and a contribution of -0.1742(19) meV to the hyperfine splitting of the 2s state in hydrogen. Distler et al. [44] give $\langle r \rangle_{(2)} = 1.045 \pm 0.004 \text{fm}$ for the 'magnetic' Zemach radius; the resulting value of $\epsilon_{Zem}$ is -0.00734, and an energy shift of -0.1676(6) meV.

The corrections due to finite size and recoil have been given in [4] as -0.145 meV, while a value of -0.152 meV is given in [70]. Combining the recoil correction from Ref. [73] with the Zemach correction results in values compatible with either of these, depending on the Zemach radius (for example, -0.1464(6) meV when the Zemach radius of Distler et al. [44] is used).

A correction for possible nuclear polarization effects has been calculated by Cherednikova et al. [71] with the result $\epsilon_{pol} = 0.00046(8)$, for an additional contribution of 0.0105 ± 0.0018 meV. Carlson et al. [73] give a value of $\epsilon_{pol} = 0.000351(114)$, or $0.0080 \pm 0.0026 \text{meV}$ for this correction. To be consistent with the recoil correction given above, the correction of Carlson et al. should be used (see also ref. [74]).

Comparable calculations for muonic deuterium and $^3$He have not been found.

In hydrogen, the total corrections (other than for the Zemach radius) amount to $0.1785 \pm 0.0027 \text{meV}$ (or $0.1762 \pm 0.0027 \text{meV}$ if the finite extent of the magnetization density in the VP correction is included). Adding $E_F$ gives 22.9839±0.0027 meV (or 22.9816±0.0027 meV). The correction due to the Zemach radius is -0.16037 meV fm$^{-1}$ $\langle r \rangle_{(2)}$. If the value of the Zemach radius from Distler et al. [44] is used, the total hyperfine splitting in the 2s-state of muonic hydrogen is 22.8140 meV.

Alternatively, one could replace the contribution from the Zemach correction by a polynomial expansion in the magnetic radius, as suggested by Carroll et al. [59]. Since the leading term in a perturbative calculation (relativistic or nonrelativistic) is linear, this should take the form $(ar + br^2)$. Since these authors take most of their radiative corrections from other work [70], which neglects some of the corrections included here, a more detailed comparison is not appropriate.

For muonic deuterium, the coefficient of $\langle r \rangle_{(2)}$ is -0.007398 fm$^{-1}$, giving, with $\langle r \rangle_{(2)} = 2.593 \pm 0.016 \text{fm}$ from [43], $\epsilon_{Zem} = -0.01918 \pm 0.00012$. Nuclear polarization and recoil corrections may be important, but have not been calculated. The total hyperfine splitting of the 2s-state, including all known corrections, is

$$\Delta E_{2s} = \frac{3}{2} \beta_D \cdot (1 + a_\mu) \cdot (1 + \epsilon_{VP} + \epsilon_{\text{vertex}} + \epsilon_{\text{Breit}} + \epsilon_{\text{Zem}}) = 6.0584(7) \text{meV}$$
For muonic $^3$He, the coefficient of $\langle r \rangle_{(2)}$ is -0.01506 fm$^{-1}$, giving, with $\langle r \rangle_{(2)} = 2.403$ fm (a Gaussian charge distribution was assumed), $\varepsilon_{Zem} = -0.0362$. The total hyperfine splitting of the 2s-state, including all known corrections, is -165.7949 meV.

**Hyperfine structure of the 2p state**

The hyperfine structure of muonic hydrogen is calculated in the same way as was done in earlier work [9, 10], but with improved accuracy. Most of the formalism and results are similar to those given by [4] and [63].

**Hydrogen**

The hyperfine structure of the 2p-state in hydrogen is given by [9, 63] ($F$ is the total angular momentum of the state)

$$
\frac{1}{4m_{\mu}m_{N}} \left\langle \frac{1}{r} \frac{dV}{dr} \right\rangle_{2p} \cdot (1 + \kappa) \left[ 2(1 + x)\delta_{jj'}[F(F+1) - j(j+1) + 3/4] + 6\hat{j}\hat{j'}(C_{F1}(1 + a_{\mu}) - 2(1 + x)) \right]
$$

where $\hat{j} = \sqrt{2j+1}$, the 6-j symbols are defined in [64], and $C_{F1} = \delta_{F1} - 2\delta_{F0} - (1/5)\delta_{F2}$.

Also

$$
x = \frac{m_{\mu}(1 + 2\kappa)}{2m_{N}(1 + \kappa)}
$$

represents a recoil correction due to Thomas precession [9, 58, 63]. For muonic hydrogen, $x = 0.0924$.

As has been known for a long time [4, 9, 10, 63], the states with total angular momentum $F = 1$ are a superposition of the states with $j = 1/2$ and $j = 3/2$. Let the fine structure splitting be denoted by $\delta = E_{2p3/2} - E_{2p1/2}$, and let $\beta' = \beta \cdot (1 + \varepsilon_{2p})$, to take the correction due to vacuum polarization into account. ($\beta$ was defined above, in Eq.14). For hydrogen, $\varepsilon_{2p} = 0.000365$ and $\beta' = 22.8138$ meV.

The energy shifts of the 2p-states with total angular momentum $F$ (notation $^{2F+1}L_j$) are then given in Table 8.

| State   | Energy       | Energy in meV |
|---------|--------------|---------------|
| $^1p_{1/2}$ | $-\beta'(2 + x + a_{\mu})/8$ | -5.9704 |
| $^3p_{1/2}$ | $(\Delta - R)/2$ | 1.8458 |
| $^3p_{3/2}$ | $(\Delta + R)/2$ | 6.3760 |
| $^5p_{3/2}$ | $\delta + \beta'(1 + 5x/4 - a_{\mu}/4)/20$ | 9.6242 |

**Table 8:** Hyperfine structure of the 2p-state in muonic hydrogen. Here $\delta = 8.352$ meV is the fine structure splitting of the 2p state.

where

$$
\Delta = \delta - \beta'(x - a_{\mu})/16
$$

$$
R^2 = [\delta - \beta'(1 + 7x/8 + a_{\mu}/8)/6]^2 + (\beta')^2(1 + 2x - a_{\mu})^2/288
$$
Some minor errors in [9] have been corrected. These numbers differ slightly from those given in ref. [3].

**Helium-3**

The formulas for muonic $^3$He are identical to those for hydrogen, but the numerical values are, of course, different. For muonic $^3$He, $x = 0.0435$, $\delta = 144.809$ meV, $\beta = -171.396$ meV

| State   | Energy       | Energy in meV |
|---------|--------------|---------------|
| $^1p_{1/2}$ | $-\beta'(2 + x + a_\mu)/8$ | 43.8458 |
| $^3p_{1/2}$ | $(\Delta - R)/2$ | -14.7877 |
| $^3p_{3/2}$ | $(\Delta + R)/2$ | 160.0510 |
| $^5p_{3/2}$ | $\delta + \beta'(1 + 5x/4 - a_\mu/4)/20$ | 135.7673 |

**Table 9**: Hyperfine structure of the 2p-state in muonic $^3$He. Here $\delta = 144.809$ meV.

$\varepsilon_{2p} = 0.000894$, and $\beta' = \beta \cdot (1 + \varepsilon_{2p}) = -171.550$ meV. The energy shifts of the 2p-states with total angular momentum $F$ (notation $^{2F+1}L_j$) are then given in Table 9.

**Deuterium**

For the 2p state, the matrix elements of the magnetic hyperfine structure have been given by Brodsky and Parsons [63]. For hydrogen they are the same as those calculated above.

The matrix elements for the magnetic hyperfine structure are then given by

$$
\begin{align*}
\varepsilon_Q &= \frac{Q}{2} \left\langle \frac{1}{r} \frac{dV}{dr} \right\rangle \\
\text{Numerically one finds, for a point Coulomb potential, and the 2p-state,} \\
\varepsilon_Q &= \frac{\alpha Q (\alpha Z m_r)^3}{24} = 0.43423 \text{ meV.}
\end{align*}
$$

As mentioned before, the Uehling potential has to be included in the potential $V(r)$. For states with $\ell > 0$ in light atoms, this can be taken into account by multiplying $\beta_D$ and $\varepsilon_Q$ by $(1 + \varepsilon_{2p})$ where $\varepsilon_{2p}$ is given by Eq. (13). With a numerical value of $\varepsilon_{2p} = 0.000391$ for muonic deuterium, the value of $\varepsilon_Q$ is increased to 0.43439 meV and the value of $\beta_D$ is increased to $\beta_D' = 4.0922$ meV.
The quadrupole interaction results in energy shifts of

\[
\begin{array}{c|cc|}
 j & j' & \text{Energy} \\
\hline
 1/2 & 1/2 & 0 \\
 3/2 & 3/2 & \epsilon_Q \left[ \delta_{F,1/2} - 4/5 \delta_{F,3/2} + 1/5 \delta_{F,5/2} \right] \\
 3/2 & 1/2 & \epsilon_Q \left[ \sqrt{2} \delta_{F,1/2} - 1/\sqrt{5} \delta_{F,3/2} \right]
\end{array}
\]

Then for the 2p-level with \( j = j' = 3/2 \) and \( F = 5/2 \), the energy shift is given by

\[
\delta + \epsilon_Q/5 + (\beta_D/40)(4 + 5x_d - a_\mu) = 9.3728 \text{ meV}
\]

For the 2p-levels with \( F = 1/2 \) and \( F = 3/2 \), the corresponding matrices have to be diagonalized. The resulting numerical values for the eigenvalues are given in Table 10.

\[
\begin{array}{c|c}
\text{State} & \text{Energy in meV} \\
\hline
^2p_{1/2} & -1.4056 \\
^2p_{3/2} & 8.6194 \\
^4p_{1/2} & 0.6703 \\
^4p_{3/2} & 8.2560 \\
^6p_{3/2} & 9.3728
\end{array}
\]

\textbf{Table 10:} Hyperfine structure of the 2p-state in muonic deuterium. Here \( \delta = 8.86419 \) meV.

Table 11 gives the contributions to the transition energies due to fine and hyperfine structure in muonic hydrogen relative to the 2s-2p\(^{1/2}\) transition energy given in Table 3.

\[
\begin{array}{c|c}
\text{Transition} & \text{Energy shift in meV} \\
\hline
^1p_{1/2} - ^3s_{1/2} & -11.6739 \\
^3p_{1/2} - ^1s_{1/2} & 18.9563 \\
^3p_{1/2} - ^3s_{1/2} & -3.8577 \\
^3p_{3/2} - ^1s_{1/2} & 23.4865 \\
^3p_{3/2} - ^3s_{1/2} & 0.6725 \\
^5p_{3/2} - ^3s_{1/2} & 3.9207
\end{array}
\]

\textbf{Table 11:} Fine- and hyperfine contributions to the Lamb shift in muonic hydrogen.

Table 12 gives the contributions to the transition energies due to fine and hyperfine structure in deuterium.

Table 13 gives the contributions to the transition energies due to fine and hyperfine structure in muonic \(^3\)He, relative to the 2s-2p\(^{1/2}\) transition energy given in Table 6.
Table 12: Fine- and hyperfine contributions to the Lamb shift in muonic deuterium.

| Transition | Energy shift in meV |
|------------|---------------------|
| $^2p_1/2 \rightarrow ^2s_1/2$ | 2.6333 |
| $^2p_3/2 \rightarrow ^2s_1/2$ | 12.6583 |
| $^4p_1/2 \rightarrow ^2s_1/2$ | 4.7092 |
| $^4p_3/2 \rightarrow ^2s_1/2$ | 12.2949 |
| $^2p_1/2 \rightarrow ^4s_1/2$ | -3.4251 |
| $^2p_3/2 \rightarrow ^4s_1/2$ | 6.5999 |
| $^4p_1/2 \rightarrow ^4s_1/2$ | -1.3492 |
| $^4p_3/2 \rightarrow ^4s_1/2$ | 6.2365 |
| $^6p_3/2 \rightarrow ^4s_1/2$ | 7.3533 |

Table 13: Fine- and hyperfine contributions to the Lamb shift in muonic $^3$He.

| Transition | Energy shift in meV |
|------------|---------------------|
| $^1p_1/2 \rightarrow ^3s_1/2$ | 85.294 |
| $^3p_1/2 \rightarrow ^1s_1/2$ | -139.134 |
| $^3p_1/2 \rightarrow ^3s_1/2$ | 26.661 |
| $^3p_3/2 \rightarrow ^1s_1/2$ | 35.705 |
| $^3p_3/2 \rightarrow ^3s_1/2$ | 201.500 |
| $^5p_3/2 \rightarrow ^3s_1/2$ | 177.216 |

Conclusions

Experimental precision has reached the point that some previously neglected effects should be taken into account. A few of these have been discussed in this paper.

The consequence of the model dependence of the coefficient of $r^3$ (in units meV fm$^{-3}$) for the determination of the nuclear radius has been discussed. The conversion of the coefficient of the third Zemach radius to $\langle r^2 \rangle^{3/2}$ is not unique. For the case of hydrogen, the contribution 0.009126 meV fm$^{-3}$ $\langle r^3 \rangle$ is most plausibly 0.0365(18) meV fm$^{-3}$ $\langle r^2 \rangle^{3/2}$. This will increase somewhat the theoretical error given in [2]. Assuming the value of the proton radius given in [2], the contribution to the transition energy would be 0.02179±0.00107 meV (here only the uncertainty in the coefficient was considered).

The radiative correction to the contribution to the energy shift of the 2s-state due to nuclear size has been included and the nuclear size contribution to the vacuum polarization correction has been calculated more completely. Details are given in Appendix B.

The previously neglected corrections to the muon Lamb shift discussed in Appendix C have not been included in the summaries. They introduce an additional theoretical uncertainty, which is of the order of 1-2 µeV for hydrogen. They are not negligible for the other cases studied here. Although the basic conclusions in the hydrogen experiment are unchanged, the theoretical uncertainty is increased, which would slightly increase the uncertainty in the determination of the proton radius.

The numerical results for muonic helium differ somewhat from those of Martynenko [76]. It is difficult to compare all terms, but Martynenko’s calculation of the Wichmann-
Kroll contribution is incorrect (the sign is wrong, for reasons described in section 9.3.1 of ref. [3]). Also, not all of the fourth order contributions to the muon Lamb shift were taken into account.

The hyperfine splitting of the 2s-state has been recalculated, including some previously neglected effects. The result for muonic hydrogen is

$$(22.9816 \pm 0.0027) \text{meV} - 0.16037 \text{meV} \cdot \langle r \rangle^2.$$  

For muonic deuterium the total hyperfine splitting of the 2s-state is

$$6.17625 \text{meV} - 0.045446 \text{meV} \cdot \langle r \rangle^2 = 6.0584(7) \text{meV}.$$  

A relativistic nonperturbative calculation of these effects is desirable, and has been performed in part [59]. Since some problems with the hyperfine structure of the 2s state have been mentioned, no further comments will be given here.

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Appendix A: Details of the relativistic recoil calculation

As mentioned before, the energy levels of muonic atoms are given, to leading order in $1/m_N$ by

$$E = E_r - \frac{B_0^2}{2m_N} + \frac{1}{2m_N} \langle h(r) + 2B_0P_1(r) \rangle$$

where $E_r$ is the energy level calculated using the Dirac equation with reduced mass and $B_0$ is the unperturbed binding energy. Also

$$h(r) = -P_1(r)(P_1(r) + \frac{1}{r}Q_2(r)) - \frac{1}{3r}Q_2(r)[P_1(r) + \frac{Q_4(r)}{r^3}]$$

where $P_1$, $Q_2$, and $Q_4$ are defined in Eq. (9). The calculation of these corrections in first order perturbation theory, and to first order in the Uehling potential, is described in detail here. It was also given in ref. [6]. Some minor mistakes in the numerical calculation have been corrected. In the case of a point Coulomb potential ($V(r) = -\alpha Z/r$), the functions $P_1$ and $Q_4$ are identically zero. The total potential considered here is $V(r) = -\alpha Z/r + V_{Uehl}(r)$.

For the contribution due to the term $B_0^2/2m_N$ the unperturbed binding energy is taken to be equal to $B_{0D} + \langle V_{Uehl} \rangle$, where $B_{0D}$ is the point Coulomb Dirac binding energy. The contribution to $B_0^2/2m_N$ that is linear in the Uehling potential is then $-B_{0D}\langle V_{Uehl} \rangle/m_N$.

Note that

$$P_1(r) + \frac{1}{r}Q_2(r) = -V(r)$$

Thus it is possible to rearrange $h(r)$ to give

$$h(r) = P_1(r)V(r) - \frac{1}{3r}Q_2(r)[P_1(r) + \frac{Q_4(r)}{r^3}]$$
As noted elsewhere in this paper (see Eq. (13)), an effective effective charge density \( \rho_{VP} \) for vacuum polarization can be derived from the Fourier transform of the Uehling potential. Recall that (for a point nucleus)

\[
V_{Uehl}(r) = -\frac{\alpha Z}{r} \frac{2\alpha}{3\pi} \cdot \chi_1(2m_e r)
\]

\[
= -\left(\frac{\alpha Z}{r}\right) \frac{2\alpha}{3\pi} \cdot \int_1^\infty \frac{dz}{z} \left(\frac{z^2 - 1}{2z^2}\right) \cdot \left(1 + \frac{1}{2z^2}\right) \cdot \left(\frac{2}{\pi} \int_0^\infty \frac{q^2 \cdot j_0(qr)}{q^2 + 4m_e^2 z^2} dq\right)
\]

where \( \chi_\pi(x) \) is defined in [1]. In momentum space, the Fourier transform of \( \nabla^2 V \) is obtained by multiplying the Fourier transform of \( V \) by \( -q^2 \). One then obtains

\[
4\pi \rho_{VP}(r) = \frac{2\alpha}{3\pi} \cdot \int_1^\infty \frac{dz}{z} \left(\frac{z^2 - 1}{2z^2}\right) \cdot \left(1 + \frac{1}{2z^2}\right) \cdot \left(\frac{2}{\pi} \int_0^\infty \frac{q^4 \cdot j_0(qr)}{q^2 + 4m_e^2 z^2} dq\right)
\]

\[
= \frac{2}{\pi} \cdot \int_0^\infty q^2 U_2(q) j_0(qr) dq
\]

(22)

\( U_2(q) \) is defined in [1] (see also Eq. (4)).

Keeping only the Coulomb and Uehling potentials, one finds

\[
P_1(r) = -\alpha Z \frac{2\alpha}{3\pi} (2m_e) \chi_0(2m_e r)
\]

\[
Q_2(r) = \alpha Z \left(1 + \frac{2\alpha}{3\pi} [\chi_1(2m_e r) + (2m_e r) \chi_0(2m_e r)]\right)
\]

\[
Q_4(r) = \alpha Z \frac{2\alpha}{3\pi} \int_1^\infty \frac{dz}{z} \left(\frac{z^2 - 1}{2z^2}\right) \cdot \left(1 + \frac{1}{2z^2}\right) \cdot \left(\frac{2}{\pi} \int_0^\infty \frac{q^2 \cdot j_0(qr)}{q^2 + 4m_e^2 z^2} dq\right)
\]

Since vacuum polarization is assumed to be a relatively small correction to the Coulomb potential, it will be sufficient to approximate \( Q_2(r)/r \) by \( \alpha Z/r \) and

\[
P_1(r)(P_1(r) + \frac{1}{r} Q_2(r)) = P_1(r) V(r) \text{ by } -\frac{\alpha Z}{r} P_1(r).
\]

Since the correction is to be calculated to linear order in the vacuum polarization potential, it will also be sufficient to use point Coulomb wave functions to calculate the expectation values. Also, for this case, one can use Schroedinger wave functions, since an accuracy of 1% will be adequate. After some algebra, one can reduce the expectation values to single integrals:

\[
\langle P_1(r) \rangle = -2m_e \alpha Z \frac{2\alpha}{3\pi} \int_1^\infty \frac{dz}{z} \left(\frac{z^2 - 1}{2z^2}\right) \cdot \left(1 + \frac{1}{2z^2}\right) \cdot \left(\frac{(az)^2 - az + 1}{1 + az} \delta_{\ell 0} + \frac{1}{(1 + az)^3} \delta_{\ell 1}\right) dz
\]

\[
\langle \frac{\alpha Z}{r} P_1(r) \rangle = -\left(\frac{\alpha Z}{r}\right)^3 m_e \frac{2\alpha}{3\pi} \int_1^\infty \frac{dz}{z} \left(\frac{z^2 - 1}{2z^2}\right) \cdot \left(1 + \frac{1}{2z^2}\right) \cdot \left(\frac{2(az)^2 + 1}{2(1 + az)^4} \delta_{\ell 0} + \frac{1}{2(1 + az)^4} \delta_{\ell 1}\right) dz
\]
with \( a = 2m_e/(\alpha Zm_r) \).

Finally,

\[
\langle \frac{\alpha Z}{3r^4} Q_4(r) \rangle = -\frac{(\alpha Z)^4 m_r^2}{6 \pi} \int_1^\infty \frac{(z^2 - 1)^{1/2}}{z^2} \cdot \left( 1 + \frac{1}{2z^2} \right) \cdot \left[ \frac{-6}{az} \frac{2+az}{1+az} - \frac{2}{az} \ln(1+az) \right] + \frac{3(az)^2 + 2az - 1}{(1+az)^3} \cdot \left[ \frac{3+az}{4(1+az)^4} \delta_{\ell 0} + \frac{1-3az - 2(az)^2}{4(1+az)^4} \delta_{\ell 1} \right] \, dz
\]

Combining these expectation values according to equations 7 and 8, one finds a contribution to the 2p-2s transition of -0.00414 meV (hydrogen) and -0.00246 meV (deuterium).

To obtain the full relativistic and recoil corrections, one must add the difference between the expectation values of the Uehling potential calculated with relativistic and nonrelativistic wave functions, giving a total correction of 0.0169 meV for muonic hydrogen. This is in very good agreement with the correction of 0.0168 meV calculated by Veitia and Puchucki \[56\]. The treatment presented here has the advantage of treating the main contribution relativistically and applying a small correction that can be calculated using first order perturbation theory. For hydrogen, a very small correction of 0.0002 meV for the Källen-Sabry contribution to the main term was included. For deuterium, one obtains a total correction of 0.0214 meV.

A similar relativistic recoil correction for finite nuclear size should be included in a relativistic calculation starting from the Dirac equation (see Ref. \[41\]). However it is automatically taken into account when the calculation is based on a generalized Breit equation, such as in Ref. \[56\].

Appendix B: Higher order contributions to the correction for finite nuclear size

If the transition energy is written in the form

\[
\Delta E_{LS} = A + B\langle r^2 \rangle + C(\langle r^2 \rangle)^{3/2}
\]

it is necessary to calculate the quantities \( A, B, \) and \( C \). Suggested values for \( C \) have been given in the text, and \( A \) can be determined from the summary tables. Here the higher order contributions to \( B \) mentioned previously are explicitly calculated for all four cases. There are several contributions and one finds

\[
B = b_a + b_b + b_c + b_d + b_e
\]

From Eq. 5, the main term in the expression for the energy shift of the 2s-state is

\[
\Delta E_{ns} = -\frac{2\alpha Z}{3} \left( \frac{\alpha Zm_r}{n} \right)^3 \langle r^2 \rangle = b_a \langle r^2 \rangle
\]

This defines \( b_a \).
Radiative corrections to the main term have been calculated by Eides and Grotch \[42\]. They contribute an additional correction of order $\alpha(Z)^5$, which amounts to

$$-\frac{2\alpha Z}{3} \left( \frac{\alpha Z m_r}{n} \right)^3 \alpha^2 Z (23/4 - 4\ln(2) - 3/4) \langle r^2 \rangle = \alpha^2 Z (5 - 4\ln(2)) \cdot b_4 \langle r^2 \rangle = b_6 \langle r^2 \rangle$$

Next, more details for the evaluation of the order $(\alpha Z)^6$ contributions to the correction for finite nuclear size to the energy of the 2s state are given.

The terms given by Friar \[41\] involving $(\alpha Z)^2 (F_{REL} + m_r^2 F_{NR})$ in equation (5) are given for $n=2$ explicitly by

$$F_{REL} = -\langle r^2 \rangle [\gamma - \frac{35}{16} + \ln(\alpha Z) + \langle \ln(m_r r) \rangle] - \frac{1}{3} \langle r^3 \rangle \frac{1}{r} + I_{2REL} + I_{3REL}$$

and

$$F_{NR} = \frac{2}{3} \langle \langle r^2 \rangle \rangle^2 [\gamma - \frac{5}{6} + \ln(\alpha Z)] + \frac{2}{3} \langle r^2 \rangle \langle r^2 \ln(m_r r) \rangle + \frac{\langle r^4 \rangle}{40} + \langle r^3 \rangle \langle 1/r \rangle + \frac{1}{9} \langle r^5 \rangle \frac{1}{r} + I_{2NR} + I_{3NR}$$

The expectation values for the various moments of the charge distribution are given in Appendix E of ref. \[41\]. Approximate values for the integrals $I_{2REL}, I_{3REL}, I_{2NR} \text{ and } I_{3NR}$ are given only for uniform and exponential charge distributions, so these extra terms, with the exception of the contribution to $F_{REL}$ that are proportional to $\langle r^2 \rangle$ were calculated for an exponential charge distribution, even if this is not completely realistic. The additional contribution proportional to $\langle r^2 \rangle$ in the finite size correction to the 2s level in equation (5) is

$$\frac{2(\alpha Z)^3}{3} \left( \frac{\alpha Z m_r}{2} \right)^3 \langle r^2 \rangle [\gamma - \frac{35}{16} + \ln(\alpha Z)] = b_c \langle r^2 \rangle$$

The remaining terms are small, but a model independent evaluation is prohibitively difficult. Numerical values are given in Tables (3,4,5,6) with the heading "remaining order $(\alpha Z)^6$".

There are two corrections due to finite nuclear size to the vacuum polarization contribution. One of these was obtained as a result of numerical integration of the expectation value of the Uehling potential, as discussed previously. It will be denoted by $b_4 \langle r^2 \rangle$ and numerical results are listed in Table \[14\]. The (small) correction arising from the Källen-Sabry potential was also included. The other correction, due to iterations, has been calculated for hydrogen by Eides et al. \[3\] and by Pachucki \[4\]. It is given by

$$\Delta E_{2s} = -\frac{4\pi \alpha Z}{3} \langle r^2 \rangle \int V_{Uehl}(r) \psi_{2s}(r) G_{2s}(r, 0) \psi_{2s}(0) d^3r$$

Ivanov and Karshenboim \[77\] have given an expression for $G_{2s}'(r, 0)$. With $x = \alpha Z m_r r = br$, it is

$$G_{2s}'(r, 0) = \frac{\alpha Z m_r^2 e^{-x/2}}{4\pi 2x} \left[ 4x (2 - x) (\ln(x) + \gamma) + 13x^2 - 6x - x^3 - 4 \right]$$

($\gamma$ is Euler’s constant). Recall that

$$\psi_{2s}(r) = \psi_{2s}(0)(1 - x/2) \exp(-x/2)$$
Then

$$\psi_{2s}(r) G'_{2s}(r, 0) \psi_{2s}(0) = \alpha Z m^2 \frac{b^3}{8\pi^2} (1-x/2) e^{-x} \left[ (1-x/2)(\ln(x) + \gamma) + \frac{13x - 6 - x^2}{8} - \frac{1}{2x} \right]$$

It is possible to show that the integral is proportional to the correction $\varepsilon_{VP2}$ to the hyperfine splitting of the $2s$-state. If one rewrites Eq.(18) in terms of $x = 2y$, one finds

$$\psi_{2s}(r) \delta_M \psi_{2s}(r) = \frac{b^3}{8\pi} \left( \frac{2}{b} \right)^3 (\alpha Z m^2 \Delta \nu_F) (1-x/2) e^{-x}$$

$$\left[ (1-x/2)(\ln(x) + \gamma) + \frac{13x - 6 - x^2}{8} - \frac{1}{2x} \right]$$

Thus

$$\psi_{2s}(r) G'_{2s}(r, 0) \psi_{2s}(0) = \frac{b^3}{8\pi \Delta \nu_F} \psi_{2s}(r) \delta_M \psi_{2s}(r),$$

and hence

$$\Delta E_{2s} = -\frac{4\pi \alpha Z}{3} \langle r^2 \rangle \frac{b^3}{8\pi \Delta \nu_F} \int V_{Uehl}(r) \psi_{2s}(r) \delta_M \psi_{2s}(r) d^3r.$$

By definition, the quantity $\varepsilon_{VP2}$ is given by

$$\varepsilon_{VP2} = \frac{2}{\Delta \nu_F} \int V_{Uehl}(r) \psi_{2s}(r) \delta_M \psi_{2s}(r) d^3r.$$

Hence

$$\Delta E_{2s} = -\frac{\alpha Z b^3 \langle r^2 \rangle \varepsilon_{VP2}}{12} = b_e \langle r^2 \rangle$$

Since the two-loop VP corrections to $\varepsilon_{VP2}$ have been calculated, they are included in $b_e$. Effectively, the one-loop correction is multiplied by approximately 1.0077. Table 14 gives numerical values of these coefficients (in meV fm$^{-2}$). The total for hydrogen differs slightly from that given in ref. [2] (-5.2262 meV fm$^{-2}$). The difference is due partly to a more precise determination of the coefficient $b_c$ and partly to the inclusion of the radiative correction ($b_b$).

|          | Hydrogen | deuterium | $^3$He | $^4$He |
|----------|----------|-----------|--------|--------|
| $b_a$    | -5.1973  | -6.0730   | -102.520 | -105.319 |
| $b_b$    | -0.00062 | -0.00072  | -0.0243 | -0.0250 |
| $b_c$    | -0.00181 | -0.00212  | -0.1275 | -0.1310 |
| $b_d$    | -0.0110  | -0.0130   | -0.3176 | -0.3297 |
| $b_e$    | -0.0165  | -0.02062  | -0.5217 | -0.5392 |
| $B_{2s}=\text{total (2s)}$ | -5.22723 | -6.10946  | -103.511 | -106.344 |
| $b(2p_{1/2})$ | -0.0000519 | -0.0000606 | -0.00409 | -0.004206 |

Table 14: Contributions to the coefficient of $\langle r^2 \rangle$ for the energy shift of the $2s$ and $2p$-states in muonic hydrogen, deuterium, $^3$He and $^4$He, in meV fm$^{-2}$.

It is interesting to note that the total coefficient of $\langle r^2 \rangle$ calculated here for $^4$He is in excellent agreement with the calculated value given in ref. [8], where the finite size
correction for $^4$He was estimated to be $-106.2 \langle r^2 \rangle + 1.4 \langle r^3 \rangle$ (in meV). An additional term proportional to the Zemach radius is discussed in the section on relativistic recoil. For $^4$He it was parametrized as $0.4 \langle r \rangle$. It is actually proportional to $\langle r \rangle^{(2)}$, and was evaluated in the section on relativistic recoil.

For $^4$He the binding energy of the $2p_{1/2}$-state is decreased by 0.0148 meV (for a radius of 1.676 fm and a Gaussian charge distribution, which is a fairly good approximation for helium, according to Friar [41]). The contribution to the fine structure is 0.0112 meV. The difference is due to the term proportional to $\langle r^4 \rangle$, which is the same for both $2p$-levels. If the radius is 1.681 fm both of these numbers are increased by 0.0001 meV. For $^3$He the binding energy of the $2p_{1/2}$-level is decreased by 0.0213 meV (for a radius of 1.966 fm). The contribution to the fine structure is 0.0158 meV.

For muonic deuterium, the first term of equation (5) would contribute $-6.0730 \langle r^2 \rangle = -(27.817 \pm 0.078)$ meV (using the value of the radius from the newest CO-DATA compilation [14]). If the radius of 2.130(3) from ref. [18] is used, this contribution is $-26.8585 \pm 0.076$ meV. Using the total coefficient from Table 14 gives $-27.718 \pm 0.076$ meV.

The term proportional to $\langle r^3 \rangle^{(2)}$ (the coefficient is $0.0112 \text{ meV fm}^{-3}$) gives a contribution of 0.382 meV or 0.417 meV, depending on the model for the charge density, and a radius of 2.14 fm. In ref. [14] it is suggested to calculate this term according to the prescription

$$\langle r^3 \rangle^{(2)} \approx 4.0(0.2)(\langle r^2 \rangle)^{3/2}$$

Using this value, one obtains 0.439(22) meV with a radius of 2.14 fm (0.433(22) meV with a radius of 2.13 fm). The last terms in Eq. (5) contribute a term proportional to $\langle r^2 \rangle$ and remaining terms. The first is $b_c \langle r^2 \rangle = -0.00966$ meV; and the remaining terms (of order $(\alpha Z)^6$) given in [41] contribute 0.00337 meV. The complete contributions are given in Table 4.

### Appendix C: Further corrections

A number of the corrections described here, in particular the ”muon Lamb shift” and the hyperfine structure of s-states, involve the expectation value of $\nabla^2 V$. Note that using the normalizations of [1, 9], one has

$$\nabla^2 V = -4\pi\alpha Z \rho$$

where $\rho$ is the nuclear charge density.

Usually $\nabla^2 V = -4\pi\alpha Z \rho(r)$ is approximated by a delta function, giving $V = -\alpha Z/r$ and

$$\langle \nabla^2 V \rangle = -4\pi\alpha Z |\psi_{ns}(0)|^2 \delta_{\ell 0} = -4Z\alpha \left( \frac{Z \alpha m_r}{n} \right)^3 \delta_{\ell 0}$$

However, the potential should be corrected for vacuum polarization due to electron loops, and, at least for s-states, for the effect of finite nuclear size. This has been done (a long time ago) [9, 65, 66, 67] for the hyperfine structure, but up to now not for the ”muon Lamb shift”.

Calculations of the correction due to a vacuum polarization insert in the external photon line for hydrogen by Pachucki [4] and by Jentschura [57] do not agree. The contribution is estimated to be at least comparable to the experimental uncertainty, so this requires further investigation. The energy shifts for at least some of the terms in this contribution as calculated by Jentschura can be compared directly. Here vacuum polarization corrections to the Bethe logarithms will not be calculated, but vacuum
polarization corrections to the expectation values of $\nabla^2 V$ and of $\frac{1}{r} \frac{dV}{dr}$ can be calculated quite easily, and a detailed numerical comparison for these parts is possible.

The largest correction to the muon self-energy graphs involves the expectation value of $\nabla^2 V$. An effective charge density $\rho_{VP}$ for vacuum polarization can be derived from the Fourier transform of the Uehling potential, and was given by Eq. (22). It is straightforward to calculate the expectation value of $4\pi \rho_{VP}(r)$. The result for hydrogen is $\langle \nabla^2 V_{VP} \rangle_{2s} = 4.4617 \times 10^{-11} \text{ fm}^{-3}$ and $\langle \nabla^2 V_{VP} \rangle_{2p} = -8.7788 \times 10^{-13} \text{ fm}^{-3}$. As a check on this calculation, the correction to the contribution of a muon loop in the external photon line to the ”muon Lamb shift” was calculated directly from the expectation value of $4\pi \rho_{VP}(r)$. It gave precisely one half of the contribution normally labeled ”mixed vacuum polarization”, which would be expected. This number has been checked independently by other authors (3). The factor 2 comes from the fact that the two loops can appear in either order. The value of $\langle \nabla^2 V_{VP} \rangle_{2s}$ turns out to be equal to $\varepsilon_{VP1}$ (see Eq. (16)) times the point Coulomb value.

An additional correction due to distortion of the wave function of the 2s-state, was given by Ivanov et al. (68) (see also (69)), and corresponds to multiplying the point Coulomb value by $\varepsilon_{VP2}$, which, as mentioned before, has the same numerical value. Strictly speaking, this correction does not correspond to a vacuum polarization insert in the external photon line, since it involves a second external photon, but it is numerically just as important as $\varepsilon_{VP1}$.

The main contribution to the muon Lamb shift has been given by (3, 4)

$$\Delta E_{LS} = \frac{Z^3 \alpha}{3 \pi m^2} \ln \left( \frac{m}{(Z\alpha)^2 m_r} \right) + \frac{3}{8} \delta_{l0} - \ln k_0(n,l)$$

Rewriting this in terms of the expectation value of $\nabla^2 V$, and including the contribution of the lowest order anomalous magnetic moment that is proportional to $\nabla^2 V$ results in

$$\Delta E_{LS} = \frac{\alpha}{3 \pi m^2} \langle \nabla^2 V \rangle \left[ \ln \left( \frac{m}{(Z\alpha)^2 m_r} \right) + \frac{5}{6} \right] - \ln k_0(n,l)$$

In this work, corrections to the Bethe logarithm will not be calculated. The contributions that can definitely be compared with ref. (57) are then

$$\Delta E_{LS,VP} = \frac{\alpha}{3 \pi m^2} \langle \nabla^2 V_{VP} \rangle \left[ \ln \left( \frac{m}{(Z\alpha)^2 m_r} \right) + \frac{5}{6} \right]$$

Calculating the energy shifts with the values calculated from Eq. (23) for $\langle \nabla^2 V_{VP} \rangle$ gave energy shifts of 0.00191 meV for the 2s state and -0.00004 meV for the 2p$_{1/2}$ state. Including the contribution from $\varepsilon_{VP2}$ increases the shift for the 2s-state to 0.00486 meV for a total contribution of -0.00490 meV. Including the effect of finite size on the Uehling potential reduced the number for the 2s state by 0.00006 meV.

In Eqs. (3.6) and (3.14) of Ref. (57) the 10/9 should be replaced by 5/6 in order to ensure consistency with Eq. (2.28). Doing that, and calculating the expression for the same pieces of Eq. (3.14) as in Eq. (23) which is
with $V_{61} = 3.09$ for the $2s$ state and $V_{61} = -0.023$ for the $2p_{1/2}$ state gives energy shifts of 0.004885 meV for the $2s$ state and -0.000036 meV for the $2p_{1/2}$ state. These numbers agree fairly well with those calculated here.

The contribution to the spin–orbit shift due to the muon’s anomalous magnetic moment, with $a_\mu = \alpha/2\pi$ can also be checked. The expression for $\frac{1}{r} \frac{dV}{dr}$ including the Uehling potential is given by Eq. (12). $\varepsilon_{2p}$ was defined as the ratio of the value of the expectation value for the Uehling potential ($\alpha Z/r^3$), and an expression is given in Eq. (13). The numerical integration is straightforward and has been checked for accuracy. The result for hydrogen is $\varepsilon_{2p} = 0.000365$. Thus, to obtain the energy shift of the $2p_{1/2}$ state, one simply has to multiply the standard value (-0.011713 meV) by $\varepsilon_{2p}$, giving $-4.275 \times 10^{-6}$ meV. Evaluating Jentschura’s Eq.(3.10), which neglected a factor $m_\mu/m_r$, gave $-3.2265 \times 10^{-6}$ meV. Correcting for the missing mass factor gave $-3.590 \times 10^{-6}$ meV.

For an estimate of the effect of nuclear size, an exponential charge density is used, mainly because all integrals can then be calculated analytically. The charge density is then

$$\rho(r) = -\frac{1}{8\pi r_0^3} e^{-r/r_0}$$

Evaluation of the expectation value gives (expanded to lowest order in $(\alpha Z m_r r_0)$)

$$\langle \nabla^2 V_C \rangle_{2s} = -\frac{(\alpha Z)^4 m_r^3}{2} \left[ 1 - 6(\alpha Z m_r r_0) + 21(\alpha Z m_r r_0)^2 \right]$$

and

$$\langle \nabla^2 V_C \rangle_{2p} = -\frac{(\alpha Z)^4 m_r^3}{2} (\alpha Z m_r r_0)^2$$

Note that $\alpha Z m_r r_0 \approx 0.00087$ for muonic hydrogen, giving a value for $(6\alpha Z m_r r_0)$ of 0.0052. As was demonstrated a long time ago [67], the correction due to finite nuclear size is probably given correctly by $2\alpha Z m_r(r_0)^2$ (here with charge density rather than with magnetization density). The expectation value of $\nabla^2 V$ for the $2p$-state is proportional to $(\alpha Z m_r r_0)^2 \approx 7.7 \cdot 10^{-7}$, and is thus much smaller. However, one finds (to linear order in $\alpha Z m_r r_0$)

$$\left\langle \frac{1}{r} \frac{dV}{dr} \right\rangle = \frac{\alpha Z (\alpha Z m_r)^3}{24} \left( 1 - \frac{9\alpha Z m_r r_0}{2} \right)$$

The finite size correction to the muon self-energy of the $2s$-state is then approximately 0.00699 meV for a Zemach radius of 1.086 fm for hydrogen. The total correction to the muon self-energy contribution (which is negative) is then 0.00207 meV, which is too small to explain the discrepancy in the measurement of the proton radius.

Since all of these corrections have also been calculated for deuterium and the helium isotopes, one can give a set of partial corrections also for these cases. Numerical values for the corrections $\varepsilon_{VP1} + \varepsilon_{VP2}$ and $\varepsilon_{Zem}$ for the four cases discussed here are given in Table 15.

Corrections to the energy shift of the $2s$-state due to these effects are summarized in Table 16. All energies are given in meV. The standard value is calculated with Eq. (23), and does not include all contributions, since corrections to the term involving the Bethe
|                  | standard value | correction (VP) | correction (size) | corrected value |
|------------------|----------------|----------------|------------------|-----------------|
| Hydrogen         | -0.91689       | -0.004924      | 0.00699          | -0.91480        |
| Deuterium        | -1.06116       | -0.00589       | 0.02035          | -1.04670        |
| $^3$He           | -15.5515       | -0.1277        | 0.5630           | -15.1162        |
| $^4$He           | -15.9455       | -0.1314        | 0.5294           | -15.5475        |

Table 15: $(\varepsilon_{VP1} + \varepsilon_{VP2})$ and $\varepsilon_{Zem}$

Appendix D: Relativistic calculation of the hyperfine structure of the 2s state

A recent paper by Carroll et al. [59] calculates the Lamb shift in muonic hydrogen relativistically and nonperturbatively. Their calculation of the magnetic hyperfine structure of the 2s-state approximates the magnetization density as a delta function. However, the magnetization density has a finite extent, and vacuum polarization has an effect on the magnetic vector potential. To estimate these effects relativistically, they will be calculated here with point Dirac wave functions. Carroll et al. do take into account perturbation of the wave function, which is also important. A completely correct calculation takes both contributions into account.

According to Eq. (40) of ref. [1], the hyperfine structure of an ns-state is given by

$$
\Delta E_{nk} = \frac{4\pi \kappa g}{\kappa^2 - 1/4} \frac{\alpha}{2m_N} \left[ F(F+1) - s_2(s_2+1) - 3/4 \right] \cdot \int_0^\infty dr \frac{r^2}{r^2} F_{nn}(r) G_{nn}(r) \cdot \int_0^r dr_N r_N^2 \mu(r_N)
$$

(24)

where $F_{nn}$ and $G_{nn}$ are the small and large components of the wave function. $n$ is the principal quantum number and $\kappa = \ell(\ell + 1) - j(j + 1) - 1/4$. Nuclear magnetic moments are given in units of nuclear magnetons, so that the proton has $g = 2(1 + \kappa_p)$. Here the magnetization density is normalized to

$$
4\pi \int_0^\infty dr_N r_N^2 \mu(r_N) = 1.
$$

The paper by Carroll et al. [59] uses the approximation $4\pi \int_0^r dr_N r_N^2 \mu(r_N) = 1$. However, the magnetization density has contributions from finite extent and from vacuum
polarization that must be taken into account. Here this will be done perturbatively, using point Dirac wave functions. The wave functions are given in the book of Akhiezer and Berestetskii [3].

For an estimate of the effect of a finite extent on the magnetization density an exponential magnetization charge density is used, mainly because all integrals can then be calculated analytically. The density is then

\[
\mu(r) = -\frac{1}{8\pi r_0^3} e^{-r/r_0}
\]

Here \( r_0 \) corresponds to the magnetic rms radius of the nucleus, and is not necessarily the same as that corresponding to the charge radius.

Vacuum polarization affects the magnetic vector potential in the same manner as it does the electrostatic potential, and the contribution to the magnetization density is thus essentially the same as Eq. 22.

\[
4\pi \rho_{VP}(r) = \frac{2\alpha}{3\pi} \cdot \int_1^\infty \frac{dz}{z^2} \left( \frac{z^2 - 1}{z^2} \right)^{1/2} \cdot \left( 1 + \frac{1}{2z^2} \right) \cdot \left( \frac{2}{\pi} \cdot \int_0^\infty \frac{q^4 \cdot j_0(qr)}{q^2 + 4m_e^2 z^2} dq \right)
\]

\[=
\frac{2}{\pi} \cdot \int_0^\infty q^2 U_2(q) G_M(q) j_0(qr) \, dq
\]

where \( U_2(q) \) is defined in [1]. See also Eq. (4). The finite extent of the magnetization density can be taken into account when the momentum space representation is used. As usual, \( G_M \) is the magnetic form factor. One then finds

\[
4\pi \int_0^r dr_N r_N^2 \mu(r_N) = 1 - e^{-r/r_0} \left( 1 - \frac{r}{r_0} - \frac{1}{2} \left( \frac{r}{r_0} \right)^2 \right) + \frac{2\alpha}{3\pi} \int_1^\infty \frac{(z^2 - 1)^{1/2}}{z^2} \cdot \left( 1 + \frac{1}{2z^2} \right) \cdot \left( 1 + 2m_e r z \right) \cdot e^{-2m_e r z} \, dz
\]

If one uses the momentum space representation, one finds for the vacuum polarization contribution

\[
4\pi \int_0^r dr_N r_N^2 \rho_{VP}(r_N) = \frac{2}{\pi} \int_0^\infty \left( \frac{\sin(qr)}{q} - r \cos(qr) \right) U_2(q) G_M(q) \, dq
\]

The expression given in Eq. 25 can be derived directly from this form if \( G_M = 1 \).

It is interesting to notice that if one were to define a "magnetic" potential according to \( \nabla^2 V_M = 4\pi \mu(r) \), then

\[
4\pi \int_0^r dr_N r_N^2 \mu(r_N) = r^2 \frac{dV_M}{dr}
\]

This permits a more transparent comparison with results obtained by other methods. It is easy to see that the vacuum polarization contribution to Eq. 25 is identical to the vacuum polarization contribution to \( Q_2(r) \) given in Appendix A.
If the HFS given by Eq. 24 is calculated using \( 4\pi \int_0^r d\tau N_2 \tau^2 \mu(r_N) = 1 \), corresponding to the first term in the expression for a finite magnetization density (Eq. 25), for the 2s-state with \( j = 1/2 \) and \( \kappa = -1 \), the result is

\[
\Delta E_{2s} = C_{2s} \left[ -\frac{N_1(N_1 + 2)}{2\gamma - 1} + \frac{N_1^2(N_1 + 1)^2}{(2\gamma + 1)^2} \right]
\]

(26)

The factor \( C_{2s} \) is defined as

\[
C_{2s} = \frac{-\alpha g \ m_r}{6m_p \ m_\mu} \frac{b^2}{4N_1(N_1 + 1)} \frac{2\gamma + 1}{\Gamma(2\gamma + 1)} \left( \frac{1 - \gamma}{2} \right)^{1/2} [F(F + 1) - 3/2]
\]

with \( \gamma = \sqrt{1 - (\alpha Z)^2} \), \( N_1 = \sqrt{2(1 + \gamma)} \), and \( b = 2\alpha Z m_r / N_1 \). A factor \( m_r / m_\mu \) has been included to account for the fact that the magnetic moment of the muon is defined in terms of the free space mass, and not the reduced mass. It was pointed out in ref. [1] that the analysis given there does not take mass corrections to the hyperfine structure into account. Similar mass corrections were made by Carroll et al. [59].

If this is expanded in powers of \( \alpha Z \), and only the leading nonvanishing terms are retained, the result is

\[
\Delta E_{2s} \approx -\frac{\alpha^2 Z g}{12m_\mu m_p} (2\alpha Z m_r / n)^3 [F(F + 1) - 3/2]
\]

Comparing this with Eq. 14, it is easy to see that the factor multiplying \( [F(F + 1) - 3/2] \) is \(-\beta/2\) if \( Z = 1 \) and \( g = 2(1 + \kappa_p) \). Thus, except for the missing factor \( 1 + a_\mu \), this is nearly the same as the standard perturbative result. Numerically, the value for the total hyperfine splitting calculated here is 22.8079 meV; this is equal to \( (1 + \varepsilon_{Breit}) \beta \) where \( \beta \) is given by Eq. 14, as expected, since the Breit correction was defined in terms of an expansion of the expression for \( \Delta E_{2s} \) given in Eq. 26 in powers of \( (\alpha Z)^2 \), as pointed out in ref. [3]. Carroll et al. obtain 22.8229 meV for this contribution, which is not corrected for distortion of the wave functions due to vacuum polarization or finite nuclear size. The additional contribution due to distortion of the wave function due to vacuum polarization calculated here (0.0744 meV) is in fair agreement with that calculated by Carroll et al. (0.0747 meV).

The magnetization density also has to be corrected for vacuum polarization. A calculation of Eq. 24 for the vacuum polarization correction to equation 25 gives for the energy shift

\[
\Delta E_{2s} = C_{2s} \frac{2\alpha}{3\pi} \int_1^\infty \left( \frac{z^2 - 1}{z^2} \right)^{1/2} \cdot \left( 1 + \frac{1}{2z^2} \right) \cdot \frac{1}{(1 + az)^{2\gamma - 1}}
\]

\[
\cdot \left[ -N_1(N_1 + 2) \left( \frac{1}{2\gamma - 1} + \frac{az}{1 + az} \right) \right.
\]

\[
+ \frac{2(N_1 + 1)^2}{(2\gamma + 1)(1 + az)} \left[ 1 + \frac{\gamma}{1 + az} \left( \frac{2az}{2\gamma + 1} - \frac{1}{2\gamma + 1} - \frac{az}{1 + az} \right) \right] \bigg] \frac{dz}{dz}
\]

where \( a = 2m_r / b \). The resulting contribution to the total hyperfine splitting of 0.0481 meV agrees very well with the perturbative value of 0.0482 meV calculated nonrelativistically.
Including the effect of finite size on the vacuum polarization contribution to the magnetization density reduced each of the nonrelativistic perturbative contributions (modification of magnetization density and perturbation of the wave function) by $-0.00114$ meV.

To estimate the effect of finite extension of the magnetization density, the integral for the $r_0$-dependent terms in Eq. 25 is evaluated. The resulting correction to the energy shift can be expanded in powers of $br_0$. If only the leading term is retained, the result is

$$\Delta E_{2s} = C_{2s}(br_0)^{2\gamma-1}\left[-N_1(N_1+2)\left(\frac{1}{2\gamma-1} + 1 + \gamma\right)\right]$$

The correction to the hyperfine structure of the 2s-state due to finite extent of the magnetization density is proportional to $(br_0)^{2\gamma-1}$; it has thus been shown to be predominantly linear in the radius, with smaller corrections with higher powers of $br_0$. Corrections due to distortion of the wave functions due to the Coulomb potential in a nonrelativistic perturbative calculation were historically approximated by using the Zemach radius (see ref. [3]). In a nonperturbative calculation, a fit to a formula that is linear plus quadratic in the radius would be a useful approach. In any case, the finite extent of the magnetization density has a dominant contribution that is linear in the radius parameter.

The value of $r_0$ is not certain. One possibility is to take $r_0 = r_{mag}/\sqrt{12}$; another is to use $r_0 = 8r_{Zem}/35$. The radius of the magnetization density is not necessarily the same as the charge radius. The magnetic radius from the Mainz experiment [17] was given as 0.777(17) fm, which has recently been modified to 0.803(17) fm. A recent determination by the group at Jefferson Laboratory [16] gives 0.867(20) fm. Numerically, one finds a reduction of the total hyperfine splitting of $-0.111$ meV if the (revised) magnetic radius from the Mainz experiment [17] is used, and $-0.120$ meV if the result from Jefferson Laboratory [16] is used. Both differ from the usual perturbative result (approximately $-0.17$ meV), for reasons that are unclear.

In any case, the correction estimated here differs significantly from the range of standard values obtained with a nonrelativistic, perturbative calculation, so that one can only say with confidence that the correction is dominated by a term linear in the radius parameter.

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