Non-perturbative Analysis of the Influence of the Proton Magnetization and Charge Densities on the Hyperfine Splitting of Muonic Hydrogen

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We investigate the influence of the spatial extent of the proton magnetization and charge densities on the 2S hyperfine splitting in muonic hydrogen. The use of a non-perturbative relativistic Dirac approach leads to corrections of 15% to values obtained from the perturbative treatment encapsulated by the Zemach radius, which surpass the next-leading order contribution in the perturbation series by an order of magnitude.

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Precise values of the hyperfine splitting of the energy levels of electronic and muonic hydrogen have long been known to be relevant to precision tests of quantum electrodynamics \[1, 2\]. Interest in the 2S state of muonic hydrogen has been strongly stimulated by the recent precision measurement of the Lamb shift transition energy \[3\]. This experiment led to the stimulating conclusion that the proton root mean square radius differs from the previously accepted value in the literature by 4.9 \(\sigma\). Determining the proton radius depended on extracting the Lamb shift of interest from the energy of the measured transition between the 2S\(^{F=2}\) and 2S\(^{F=1}\) states. This extraction relied on a variety of mainly perturbative calculations performed by many authors, including those of Martynenko [4], Borie [5, 6], Pachucki [7, 8], and many others [9, 10, 11]. Our focus here is on the hyperfine splitting between the 2S states with total spin \(F = 1\) and \(F = 0\). A computed value (22.8148(78) meV \[4\]) was used in \[2\]. As a guide to the importance of precision, we note that a change in this value of 1% would correspond to a shift by 1\(\sigma\) in the proton radius. Furthermore, this transition is under current experimental investigation, with an announcement of a result expected soon.

The \(F = 0\) and \(F = 1\) levels of atomic \(S\) states are split by the interaction between the magnetic dipole moments of the lepton and proton. Fermi computed this splitting treating the lepton and proton as point-like particles having magnetic moments but no spatial extent, and using the Coulomb potential to compute the non-relativistic hydrogen wave function. This first-order treatment gives the Fermi energy of the \(nS\) states:

\[
E_F^{\text{(nS)}} = \frac{8}{3\hbar^2} \frac{\mu_p m_F^2 M_p^2}{(m_p + M_p)^3}, \tag{1}
\]

where \(\mu_p = 2.792847351\) is the proton magnetic moment, \(\alpha\) is the fine structure constant, and \(M_p, m_p\) denote values of the proton and muon masses. Zemach \[14\] included the influence of the spatial extent of the proton charge and magnetization distributions using first-order perturbation theory. The relevant spin-spin interaction is given by

\[
V_{\text{Zemach}} = \frac{8\pi\alpha\mu_p \tilde{\sigma}_1 \cdot \tilde{\sigma}_2 \rho_M(r)}{12m_p M_p}, \tag{2}
\]

where the scalar product of the lepton and proton Pauli matrices, \(\tilde{\sigma}_1 \cdot \tilde{\sigma}_2\) is +1 in the \(F = 1\) state and -3 in the \(F = 0\) state, and \(\rho_M\) is the magnetization density normalized to unity. A contribution of the muon anomalous magnetic moment is treated as a further (0.1%) correction as per Ref. \[4\] to which we compare. Zemach treated the difference between using \(V_{\text{Zemach}}\) and the corresponding interaction obtained by taking the magnetization density to be a delta function at the origin. His result can be expressed as

\[
\Delta E_Z = E_F \frac{2\mu \alpha}{\pi^2} \int \frac{d\tilde{p}}{\tilde{p}^2} \left[ \frac{G_F(-\tilde{p}^2)G_M(-\tilde{p}^2)}{\mu_p} - 1 \right] = E_F(-2\mu\alpha)R_p, \tag{3}
\]

where \(R_p\) denotes the appropriately-named Zemach radius of approximate value \(R_p = 1.040(16)\) fm \[4\] and \(\mu\) denotes the reduced muon mass. The appearance of \(G_F\) results from its influence on the bound-state wave function at the origin and \(G_M\) enters directly in the interaction. Effects of the spatial extent of the magnetization...
density and higher order effects of $G_M \neq 1$ are not included.

Our aim here is to treat the effects of $V_{\text{Zemach}}$ exactly within the framework of very precise numerical solutions of the two separate $F = 0$ and $F = 1$ Dirac equations. The dominant binding interaction is taken to be the sum of the Coulomb potential and its lowest-order correction arising from vacuum polarization, each being modified by the non-zero spatial extent of the proton \cite{12}. Since the size of the hyperfine splitting is much less than the size of the Lamb shift, a high degree of numerical accuracy is required. The method we use to do this is detailed in a previous publication \cite{10}. These high-precision calculations have been shown \cite{10, 13} to reproduce exact, analytic eigenvalues for a point-Coulomb potential and to satisfy a virial theorem test to within 0.5 $\mu$eV which we set as an upper bound on our numerical errors here.

To proceed we need to specify the magnetization density $\rho_M$ and corresponding magnetic radius $(r_M^2) \equiv \int d^3r \, r^2 \rho_M(r)$ (while including the effects of the charge radius $(r_C^2)$ in the dominant binding potentials). The magnetization density is taken to be a normalized exponential

$$\rho_M(r) = \frac{\eta}{8\pi} e^{-\eta r}; \quad \eta = \sqrt{12/(r_M^2)\text{M}}. \quad (4)$$

The astute reader will question whether this exponential form is a suitable choice for the magnetization density. While the dependence of the Lamb shift energy on the shape of the charge distribution has been fully investigated in Ref. \cite{10}—and discounted—this conclusion does not automatically extend to the magnetization density, which appears un-integrated in Eq. (2), as opposed to the integrated appearance in the finite-Coulomb and finite vacuum polarization potentials \cite{13}. We shall return to this issue, but for now an exponential form shall be assumed.

We calculate the converged eigenvalues for the $2S$ hyperfine splitting (being the difference between the eigenvalues for the $F = 0$ and $F = 1$ hyperfine states) by numerically integrating the Dirac equation

$$\frac{d}{dr} \left( \begin{array}{c} G_{2S}(r) \\ F_{2S}(r) \end{array} \right) = \left( \begin{array}{cc} -\kappa_{2S}/r & \lambda_{2S} + 2\mu - V \\ -\lambda_{2S} + V & \kappa_{2S}/r \end{array} \right) \left( \begin{array}{c} G_{2S}(r) \\ F_{2S}(r) \end{array} \right) \quad (5)$$

for which $\kappa_{2S} = -1$, $\mu$ again denotes the reduced muon mass, and $\lambda_{2S}$ denotes the $2S$ eigenvalue shifted by the reduced mass. In doing so we obtain the upper and lower components ($G_{2S}(r)$ and $F_{2S}(r)$, respectively) of the muon wave-function in the combination, $V$ of the finite-size Coulomb potential, finite-size vacuum polarization potential, and potential given by Eq. (2) (separately for each value of $\vec{s}_1 \cdot \vec{s}_2$), for a variety of values of $r_C^2$ and $r_M^2$.

We express the computed hyperfine splittings (HFS) as a polynomial function of $r_M^2$ for two significant choices of $r_C^2$—the 2006 CODATA \cite{17} value $r_C^2 = 0.8768$ fm (recently updated, as per NIST) and that found in the analysis of Pohl et al. \cite{8}, $r_C^2 = 0.84184$ fm. This yields

$$\Delta E_{2S}^{\text{HFS}} = A + B((r_M^2)/M) + C((r_M^2)/M)^{3/2}, \quad (6)$$

for which the values of $A$, $B$, and $C$ are given in Table I for parameterizations at the two values of $r_M^2$.

The two parameterizations are compared in Fig. 4 in which we note that the dependence on $r_M^2$ is almost nonexistent, while the dependence on $r_C^2$ is stronger. Also shown in Fig. 4 are the magnetic radii from Refs. \cite{18, 19} corresponding to the extractions from the Mainz (0.777 $\pm$ 0.029 fm) and Jefferson Laboratory (0.850 $\pm$ 0.030 fm) collaborations, respectively.

The large difference between extracted magnetic radii does not heavily influence the HFS. The difference between using the Mainz value and the JLab value is only 0.35 $\mu$eV for the smaller value of the charge radius and 0.23 $\mu$eV for the larger value. Therefore, we can average the HFS obtained from the two values of the magnetic radius to calculate the value of the $2S$ hyperfine shift for each of the value of charge radius. The results are

$$\Delta E_{2S}^{\text{HFS}} = 22.6384 \text{ meV if } r_C^2 = 0.84184 \text{ fm}$$

$$= 22.6347 \text{ meV if } r_C^2 = 0.8768 \text{ fm}. \quad (7)$$

This is the value of the $2S$ hyperfine shift obtained using a complete treatment of the spatial extent of the proton’s electromagnetic distributions. We can determine the importance of our complete treatment as compared to using only the Zemach radius by computing the $2S$ hyperfine shift in the presence of only the finite-size Coulomb and finite-size vacuum polarization potentials, which we also fit to a polynomial form to give

$$\Delta E_{2S}^{\text{HFS}} = 22.8521 - 0.1795 (r_M^2)/C + 0.0739 (r_M^2)/C^3 \text{ meV}, \quad (8)$$

as per Ref. \cite{17}. For the two chosen values of $r_C^2$ this leads to an uncorrected (with respect to the finite size of

| Table I: Coefficients of Eq. (4) parameterizing the 2S HFS with magnetic radius, relevant to the Zemach correction for two values of the rms charge radius, calculated using the finite-Coulomb ($V_{\text{FC}}$), finite vacuum polarization ($V_{\text{FVP}}$), and magnetization potentials ($V_{\text{Zemach}}$); and alternatively the finite-Coulomb potential plus magnetization potential. |
|-----------------|-----------------|-----------------|-----------------|
| $r_M^2$         | $A$ [meV]       | $B$ [meV fm$^{-2}$] | $C$ [meV fm$^{-3}$] |
|-----------------|-----------------|-----------------|-----------------|
| 0.84184         | 22.6085         | 0.1425          | -0.1191         |
| 0.8768          | 22.6037         | 0.1450          | -0.1203         |
| 0.8768          | 22.5318         | 0.1388          | -0.1142         |
| \[a\] Calculated using $V = V_{\text{FC}} + V_{\text{FVP}} + V_{\text{Zemach}}$ |
| \[b\] Calculated using $V = V_{\text{FC}} + V_{\text{Zemach}}$ |
FIG. 1: Comparison of data and parameterizations of Zemach corrections to the 2S hyperfine state of muonic hydrogen for two values of the proton rms charge-radius. Also shown are the calculated fits (‘Fit 1’ and ‘Fit 2’ denote fits for \( r_p^C = 0.84184 \) fm and \( r_p^C = 0.8768 \) fm respectively) to the data as presented in the first two lines of Table I and the magnetic radii extracted from Bernauer et al. [18] [Mainz, \( \langle r^2_{M} \rangle^{1/2} = 0.777 \pm 0.029 \) fm] and Gilad et al. [19] [Jefferson Lab Hall A Collaboration, \( \langle r^2_{M} \rangle^{1/2} = 0.850 \pm 0.030 \) fm] used to calculate the Zemach corrections of Eq. (7). The point denoted by a star corresponds to the Zemach correction calculated via charge and magnetization densities extracted from Ref. [20] at \( r_p^C = 0.878 \) fm and \( r_p^M = 0.860 \) fm as per Eq. (17).

The isolated Zemach correction calculated here is given by the difference between the corrected calculation and the uncorrected one,

\[
\Delta E_{Zemach} = \Delta E_{HFS}^{2S} - \Delta E_{HFS}^{2S,\text{Z}}.
\]

(9)

The proton magnetization distribution) HFS of \( \Delta E_{2S}^{HFS} \) is

\[
\begin{align*}
\Delta E_{2S}^{HFS} & = \begin{cases} 
22.7690 \text{ meV} & \text{if } r_p^C = 0.84184 \text{ fm} \\
22.7639 \text{ meV} & \text{if } r_p^C = 0.8768 \text{ fm}
\end{cases}.
\end{align*}
\]

(10)

In order to identify the significance of vacuum polarization on this result, we furthermore recalculate the Zemach correction using only the finite-size Coulomb potential plus potential given by Eq. (2). In this case, calculating the potentials using \( r_p^C = 0.8768 \) fm for various values of \( r_p^M \) we obtain a polynomial of the form given by Eq. (6) with values of \( A, B, \) and \( C \) listed in the last line of Table I. Using this polynomial form we calculate the HFS contribution for the two values of \( r_p^M \) and average (though they are separated by only twice our numerical error) to obtain

\[
\Delta E_{2S}^{HFS,\text{Z}} = 22.5621 \text{ meV}.
\]

(11)

We may compare this to the uncorrected shift calculated using only the finite-Coulomb potential in Ref. [15], interpolated to \( r_p^C = 0.8768 \) fm, and we obtain

\[
\Delta E_{2S}^{HFS} = 22.6910 \text{ meV},
\]

(12)

indicating a correction using the finite-Coulomb potential alone (neglecting the vacuum polarization) of

\[
\Delta E_{Zemach} = -0.1289 \text{ meV}.
\]

(13)

The deviation of this value from that in Eq. (10) for the same value of \( r_p^C \) is a mere 0.3 \( \mu \)eV, indicating that vacuum polarization has negligible influence on the Zemach correction within our numerical error limits.

Returning to the issue of the significance of the shape of the various distributions used in these calculations, we have recalculated the Zemach correction using charge and magnetization densities extracted from fits to form-factor data [20] explicitly. The so-called charge and magnetization densities \( \rho_{C,M}(r) \) may be extracted from the Sachs electric and magnetic form factors \( G_{E,M}(Q^2) \) via a Fourier transform

\[
\rho_{C,M}(r) = \int \frac{d^3 q}{(2\pi)^3} e^{-i\vec{q}\cdot\vec{r}} G_{E,M}(\vec{q}^2),
\]

(14)

where for an atomic system we have \( Q^2 = q^2 \), and we take the Sachs form factors as the fits given in Ref. [20].
of the form

\[ G_E(Q^2) = \frac{1 + q_6 r + q_{10} r^2 + q_{14} r^3}{1 + q_2 r + q_4 r^2 + q_6 r^3 + q_{12} r^4 + q_{16} r^5}, \]  

(15)

\[ G_M(Q^2) = \frac{1 + p_6 r + p_{10} r^2 + p_{14} r^3}{1 + p_2 r + p_4 r^2 + p_6 r^3 + p_{12} r^4 + p_{16} r^5}, \]  

(16)

(noting that the proton magnetic moment \( \mu_p \) appears in Eq. (2) here rather than in \( G_M \) with coefficients \( q_i \) and \( p_i \) given in Table II and for which \( r = Q^2/4M_r^2 \)) Using the extracted charge density in the finite-Coulomb potential (which as per Ref. 24 is constrained such that \( r_p^C = 0.878 \) fm), and the extracted magnetization density (constrained such that \( r_p^M = 0.860 \) fm) in the Zemach potential (the finite vacuum polarization potential, which as noted before is of minimal consequence, remains calculated using an exponential charge distribution characteristic of \( r_p^C = 0.8768 \) fm), we once again recalculate the Zemach correction to the 2S HFS, and we find

\[ \Delta E_{\text{HFS,Z}}^{2S} = 22.6335 \text{ meV}. \]  

(17)

As we do not have knowledge of either the \( r_p^C \) or \( r_p^M \) polynomial dependence of this energy, we may only compare to an interpolation of our previous results at the appropriate values. Comparing Eq. (17) to our polynomial fit corresponding to \( r_p^C = 0.8768 \) fm (the difference in \( r_p^C \) being minimal) as per the second line of Table II and interpolating to \( r_p^M = 0.860 \) fm, we find a difference of a mere 1.0 \( \mu \)eV, indicating that the exponential distribution is indeed a good approximation for the magnetization density. This Zemach corrected HFS is included in Figure I where it is clear that it produces good agreement with our usage of a simplified model of the charge and magnetization densities.

We compare our values of the Zemach correction (Eq. (10) and Eq. (13)) to that which was used in the analysis of Pohl et al. 5, viz. that of Martynenko 4 (denoted in that reference as ‘Proton structure corrections of order \( \alpha^5 \))

\[ \Delta E_{\text{Zemach}} = -0.1518 \text{ meV}. \]  

(18)

This includes the influence of the Zemach term as well as the small (\( \sim 5 \% \)) on the value of the Zemach radius) effects of a putative treatment of the two-photon exchange interaction (with intermediated nucleon states).

The comparison between Eq. (10) and Eq. (13) suggests that the value used in the analysis of Pohl et al. requires a significant modification of some 10–15%. A more precise consideration of the importance of using a complete non-perturbative treatment is to look at the next-leading contribution of Ref. 4 (‘Proton structure correction of order \( \alpha^6 \) = -0.0017 meV). This is an order of magnitude smaller than the difference found here, indicating that the perturbative approach is not satisfactory in this scenario.

We may also study the importance of the Zemach radius by examining the values of the Zemach radii for the values of \( r_p^C,M \) of present interest, as displayed in Table III. The HFS is almost independent of the value of \( r_p^M \), but the Zemach radius displays a very significant dependence on this parameter.

The difference between our value quoted in Eq. (10) and the value of Martynenko quoted in Eq. (13) does not resolve the proton radius puzzle. The effect presented here alters the 2S hyperfine splitting by 0.02 meV, contributing only 0.005 meV (while 0.3 meV is needed) to the transition measured by Ref. 5. However, our results add weight to the argument that the perturbative corrections require further attention and re-evaluation using the latest numerical tools, along with a close examination of the relevant physics to ensure that no contribution is overlooked, such as that reported in Ref. 21.

Recomputing the 2S HFS with this new Zemach inclusion, we obtain a splitting as given in Table IV which summarizes our updated non-perturbative calculation of this splitting.

We note a relevant error in Ref. 13—the Zemach contributions to the 2S HFS labelled ‘Proton structure corrections of order \( \alpha^5 \)’ and \( \alpha^6 \) are listed in Table III of Ref. 13 as included by the Dirac calculation, whereas

| \( r_p^C \) | \( R_p \) (fm) | \( R_p \) (fm) | \( R_p \) (fm) |
|---|---|---|---|
| 0.84184 | 1.022 | 1.068 |
| 0.878 | 1.046 | 1.091 |
| 0.878 | 1.081 |
these terms should appear under ‘Remaining corrections’. This contribution now appears corrected in Table IV which should serve as a replacement to the former table. The re-calculation of the Zemach contribution alters the prediction of the proton rms radius via the analysis of Ref. [15] to arrive at

\[ r_p^C = 0.84182(67) \text{ fm}, \]  

which does not differ from the former conclusion \((r_p^C = 0.83811(67) \text{ fm})\) in a statistically significant fashion with regard to the main discrepancy, but does agree with that of Pohl et al. to a high level of precision.

We conclude by stating that our calculation of the influence of the spatial extent of the proton’s electromagnetic distributions using a non-perturbative, relativistic framework results in a 10–15% deviation of the Zemach correction from the value used by Pohl et al. Furthermore, the very weak dependence of the HFS on the value of the magnetic radius, shows that the perturbative treatment, dominated by the influence of the Zemach radius, does not capture the effects of the proton’s spatial distributions on the HFS. This result invites and encourages further investigation into the many corrections which enter the analysis of the muonic hydrogen spectrum at the level of precision required to extract the value of the proton radius at the required level of precision.

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TABLE IV: Contributions to the $2S_{1/2}$ hyperfine splitting with comparison to values found in Martynenko [3] corrected and updated from Ref. [15] to include the re-calculated Zemach contribution. Values are all in meV. Errors in the Dirac calculations are taken to be $\pm 500$ neV. The listed corrections are already included in our Dirac calculations and are listed by their descriptions in Ref. [4]. All further corrections to both the perturbative calculation and our calculation are contained in 'Remaining Corrections' which encompasses the muon AMM, amongst other corrections listed in Ref. [4]. We note that the in Ref. [4] the Zemach correction is listed as ‘Proton structure corrections of $O(\alpha^5)$’ and may not include considerations of finite-size in the wave-function. The polynomial dependence on $(r_p^2)^n$ of this splitting is not discussed in the literature. The strict $r_p^C$ dependence of the Zemach correction has not been calculated, and as such we have selected a value (that corresponding to $r_p^C = 0.8768$ fm) suitable to our previous analysis [15].

| Contribution                                      | Martynenko | Present Work |
|--------------------------------------------------|------------|--------------|
| Dirac ($V = V_C$)                                | 22.8229    |              |
| Dirac ($V = V_C + V_{VP}$)                       | 22.8976    |              |
| Dirac ($V = V_{FC}$)                             | 22.7774 - 0.1746 $\langle r_p^2 \rangle + 0.0709 \langle r_p^2 \rangle^{3/2}$ |              |
| Dirac ($V = V_{FC} + V_{VP}$)                    | 22.8510 - 0.1701 $\langle r_p^2 \rangle + 0.0667 \langle r_p^2 \rangle^{3/2}$ |              |
| Dirac ($V = V_{FC} + V_{FVP}$)                   | 22.8521 - 0.1795 $\langle r_p^2 \rangle + 0.0739 \langle r_p^2 \rangle^{3/2}$ |              |
| Fermi Energy $E_F$                               | 22.8054    |              |
| Relativistic correction $\frac{4Z}{3}(Z\alpha)^2E_F$ | 0.0026     |              |
| VP corrections of orders $\alpha^5$, $\alpha^6$  |            |              |
| in the second order of perturbation series       | 0.0746     |              |
| Proton structure corrections of order $\alpha^5$ | -0.1518    |              |
| Proton structure corrections of order $\alpha^6$ | -0.0017    |              |
| Zemach correction                                | -0.1292    |              |
|subtotal:                                        | 22.7291    | 22.7229 - 0.1795 $\langle r_p^2 \rangle + 0.0739 \langle r_p^2 \rangle^{3/2}$ |
| Remaining Corrections                            | 0.0857     | 0.0857       |
|total:                                           | 22.8148 $\pm$ 0.0078 | 22.8086 - 0.1795 $\langle r_p^2 \rangle + 0.0739 \langle r_p^2 \rangle^{3/2}$ |