Non-Perturbative Relativistic Calculation of the Muonic Hydrogen Spectrum

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We investigate the muonic hydrogen $2P_{3/2}^F$ to $2S_{1/2}^F$ transition through a precise, non-perturbative numerical solution of the Dirac equation including the finite-size Coulomb force and finite size vacuum polarization. The results are compared with earlier perturbative calculations of (primarily) Borie, Martynenko, and Pachucki \textsuperscript{1, 2, 3} and experimental results recently presented by Pohl et al. \textsuperscript{4}, in which this very comparison is interpreted as requiring a modification of the proton charge radius from that obtained in electron scattering and electron hydrogen analyses. We find no significant discrepancy between the perturbative and non-perturbative calculations, and present our results as confirmation of the perturbative methods.

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I. INTRODUCTION

The precision measurement of the Lamb shift transition energy between the $2P_{3/2}^F$ and $2S_{1/2}^F$ states of muonic hydrogen by Pohl et al. \textsuperscript{4}, see Fig. 1, has created considerable interest because of a 0.31 meV discrepancy with the value predicted by theoretical calculations (specifically those discussed in Ref. 7; Borie \textsuperscript{1, 2, 3} and Martynenko \textsuperscript{4, 5} along with many others \textsuperscript{8–11}). This Lamb shift splitting of $\mathcal{O}(206)$ meV is dominated by the lowest order QED vacuum polarization, and obtains a significant contribution from the finite size of the proton. On selecting and combining the perturbative predictions for the corresponding contributions to the measured transition, Pohl et al. produce a cubic equation relating their experimentally measured energy shift to the theoretical prediction, and arrive at

$$206.2949(32) \text{ meV} = 206.0573(45)$$
$$-5.2262\langle r_p^2 \rangle^{1/2}$$
$$+0.0347\langle r_p^3 \rangle^{3/2} \text{ meV,} \quad (1)$$

the only physically-meaningful solution of which implies a proton rms charge radius of $r_p \equiv \sqrt{\langle r_p^2 \rangle} = 0.84184(67)$ fm which differs from the consensus CODATA \textsuperscript{12} value of $r_p = 0.8768(69)$ fm by 4.9 standard deviations.

Such a large modification of a basic electromagnetic property of the proton suggests that either there may be an as yet unrecognised problem in several other experimental efforts (such as the electronic hydrogen spectroscopy and scattering experiments which primarily lead to the CODATA value \textsuperscript{12}) or in the QED calculations \textsuperscript{13, 14}, or alternatively that some new physics (beyond the Standard Model) contributes to this transition energy \textsuperscript{15, 16}. With respect to the QED calculations, we note that the predominant theoretical approach involves perturbation theory applied to the solutions of the non-relativistic Schrödinger equation \textsuperscript{1, 4, 5}. Since the effects of finite size and the vacuum polarization potential are quite large at short distance, it seems important to verify by explicit calculation that the perturbative treatment is indeed adequate at the level quoted.

We therefore calculate the transition energy relevant to the aforementioned experiment using the relativistic Dirac equation to describe the muon wave function non-perturbatively. We take care to control the numerical errors in the calculations and to quantify any differences from the perturbative non-relativistic approach. In our work we extend considerably the earlier work by Borie \textsuperscript{1, 2}.

In the sections following, we discuss the nature of the transition and contributing physical effects, as well as the method by which we calculate the energies corresponding to the various eigenstates. We summarize any discrepancies with respect to previous work.

II. MUONIC HYDROGEN SPECTRUM

After muon capture by hydrogen, about 1% of the muons reach the metastable $2S$-state. This state is activated by laser excitation from $2S_{1/2}$ to $2P_{3/2}^F$ and the signature that the laser energy is well tuned is the appear-
ance of a prompt E1 transition X-Ray of a muon from the 2P_{3/2} state of muonic hydrogen to the 1S_{1/2} state. Given the resonance method used to establish the energy of the Lamb shift, there appears to be no doubt about the remarkable experimental result of Pohl et al. [7].

The L-shell level scheme explored in this experiment is depicted in Fig. 1 for the point-Coulomb potential of magnitude

$$V_C(r) = -\frac{Z\alpha}{r}. \quad (2)$$

The 2S_{1/2} and 2P_{1/2} states are degenerate even in the Coulomb-Dirac theory. Since the muon orbit is 200 times smaller than the corresponding electron orbit, the S-states probe the point charge smearing effect of vacuum polarization, which is the dominant component in the Lamb shift, $\Delta E^{2S-2P}_\text{Lamb}$, in Fig. 1. Of similar nature is a smaller but significant effect for hydrogen ($Z = 1$) arising from the finite proton charge radius, denoted $\Delta E^{2S}_\text{Finite}$ in Fig. 1. While the vacuum polarization effect increases the binding of the S_{1/2} states pulling these ‘down’ in Fig. 1, the finite charge distribution acts in the opposite direction.

The spin-orbit fine structure splitting of the 2P_{1/2} and 2P_{3/2} eigenstates is predicted by the Dirac equation. It is denoted by $\Delta E^{2P}_\text{FS}$ in Fig. 1. As the measured transition does not involve the 2P_{1/2} state, we shall only calculate the relevant energy levels for the purpose of comparison with perturbative results.

The spin-spin coupling of the muon to the proton adds hyperfine splitting to the spectrum. For the case of the 2S_{1/2} eigenstate, this leads to hyperfine eigenstates with total angular momenta $F = 0$ and $F = 1$. The muon involved in the measured transition decays to the 2S_{F=1} state, and thus we address an accurate determination of the energy of this state and the corresponding splitting $\Delta E^{2S}_\text{HFS}$. Similarly, the hyperfine states are labeled by $F = 0$ and $F = 1$ for the 2P_{1/2} case, and $F = 1$ and $F = 2$ for the 2P_{3/2} case. The hyperfine splitting energies are denoted here by $\Delta E^{2P_{1/2}}_\text{HFS}$ and $\Delta E^{2P_{3/2}}_\text{HFS}$ for the corresponding states. The muon in the measured transition decays from the 2P_{3/2} eigenstate, so we require an accurate determination of the energy of this state. We note that the muon-proton tensor force does lead to some mixing of the two F=1 states but we will not make a new calculation of this effect.

III. NUMERICAL METHOD

To calculate the theoretical energy difference corresponding to the measured transition, previous authors have primarily used perturbation theory with non-relativistic wave functions, including in the effective interaction terms describing the various relativistic corrections. In order to calculate the perturbative effect on the energy produced by an operator, $\delta V$, additional to the Coulomb potential,

$$V_{\text{eff}} = -\frac{Z\alpha}{r} + \delta V, \quad (3)$$

we require a wave function to integrate over. If we follow the methods of previous authors, we can use exact Schrödinger wave functions for states with quantum numbers $n, \ell, m$ and the lowest order correction to the energy is

$$\Delta E^{n\ell m}_\text{V} \approx \int_0^\infty \phi_{\text{Schrod}}^{n\ell m}(r) \delta V \phi_{\text{Schrod}}^{n\ell m}(r) d^3r. \quad (4)$$

An alternate approach, which we choose here, is to use the Dirac equation with the appropriate potential in order to calculate the perturbed wave functions. This approach is known to be a specific limit approximation to the two-particle Bethe-Saltpeter equation [8].

We consider the muon wave function in state $\alpha$ to be a spinor $\psi_\alpha(\vec{r})$

$$\psi_\alpha(\vec{r}) = \begin{pmatrix} g_\alpha(r) \chi_+^\alpha(\hat{r}) \\ -if_\alpha(r) \chi_-^\alpha(\hat{r}) \end{pmatrix} = \begin{pmatrix} G_\alpha(r) \\ -iF_\alpha(r) \end{pmatrix} \begin{pmatrix} \chi_+^\alpha(\hat{r}) \\ \chi_-^\alpha(\hat{r}) \end{pmatrix}, \quad (5)$$

normalised to unity, such that the probability is

$$\int |\psi_\alpha|^2 d^3r = \int_0^\infty r^2 \left[ g_\alpha(r)^2 + f_\alpha(r)^2 \right] dr = 1, \quad (6)$$

noting that $\chi_\kappa^\alpha$ are eigenfunctions of the total angular momentum operator (consisting of a combination of spheri-
cal harmonics and Pauli spinors) satisfying
\[
\int \lambda_{\alpha}^{m_1} \lambda_{\kappa}^{m_2} d\hat{r} = \delta_{\alpha\kappa} \delta_{m_1 m_2}.
\] (7)

The separation of center of mass motion is not exact for a relativistic two body system. To lowest order in the ratio of muon to proton mass we use the reduced mass \(\mu\) in place of the muon mass in the Dirac Equation
\[
\mu = \frac{M_p m_\mu}{M_p + m_\mu}.
\] (8)

Along with further recoil corrections treated in perturbation theory, this should provide a very accurate description of the system.

The binding of the muon in this system is extremely sensitive to the overall center-of-mass motion. To convince ourselves that our method is self-consistent, we check the accuracy of our procedure using several methods. The unperturbed point-Coulomb Dirac eigenvalues are known analytically to be
\[
\lambda_\alpha = \epsilon_\alpha - \mu = \mu \left[ 1 + \frac{Z^2 \alpha^2}{(n_\alpha - |\kappa_\alpha| + \sqrt{\kappa_\alpha^2 - Z^2 \alpha^2})^2} \right]^{-\frac{1}{2}} - \mu,
\] (10)

where \(n_\alpha\) denotes the principle quantum number for state \(\alpha\). We first ensured that were are able to reproduce these values with a reasonable compute-time. For the 2S_{1/2} wave function, we reproduce the analytic result to within 10 neV, the 2P_{3/2} eigenstate to within 40 neV and the 1S_{1/2} and 2P_{3/2} eigenstates to within 10 neV, using precision Fortran, a sufficiently large grid size, and sufficiently small grid spacing.

This test does not assure that solutions for a realistic system—including the finite size of the proton as well as finite size vacuum polarization—converges with same accuracy. For this reason we employ the virial theorem, and test for our solutions (refer to Ref. [6] for further details) by calculating the reduced eigenvalue as
\[
\lambda_\alpha = \langle \psi_\alpha | \mu (\beta - 1) + V(\mathbf{r}) + \mathbf{r} \cdot \nabla V(\mathbf{r}) | \psi_\alpha \rangle.
\] (11)

The virial theorem provides a far more stringent test of the accuracy of the muon wave function near the origin, where \(|\nabla V|\) is greatest. We find that the eigenvalues calculated using Eq. (11) and Eq. (13) for the 2S_{1/2} wave function differ by 180 neV for a point-Coulomb potential, and 450 neV the finite-Coulomb plus finite-vacuum polarization potentials discussed in Sec. [VI]. We therefore conservatively take our errors to be less than \(\pm 500\) neV. Propagating this error, we find that in principle we could determine the required proton rms charge-radius to within approximately 0.05 am (\(5 \times 10^{-5}\) fm). This should be sufficient to provide a reliable, independent test of the accuracy of the perturbative approach, however we note that the determination of the proton rms charge radius cannot be performed to this precision as the error in that analysis is dominated by experimental error in the determination of the transition energy.

V. 2S_{1/2}-2P_{3/2} LAMB SHIFT

The Lamb shift is the splitting of the otherwise degenerate 2S_{1/2} and 2P_{3/2} eigenstates attributed to the vacuum polarization potential \(V_{VP}\), which for a point source is given in [6] as
\[
V_{VP}(r) = -\frac{Z \alpha}{r} \frac{e^{-m_e q r}}{3 \pi} \int_0^\infty \frac{1}{q^2} \sqrt{1 - \frac{4}{q^2}} \left( 1 + \frac{2}{q^2} \right) dq^2,
\] (12)

where \(m_e\) is the electron mass. We can calculate the effect that this has on the eigenvalues by assuming that this potential is a small perturbation of the Coulomb potential, and thus using Eq. (11) we find
\[
\Delta E_{Lamb}^{\ell m} \approx \int_0^\infty V_{VP}(r) |\psi_{Schr.}^{\ell m}(r)|^2 d^3r,
\] (13)
to which we must also add higher order perturbation theory, relativistic, recoil, and radiative corrections and generally higher-order (in \(\alpha\)) corrections.

Alternatively—and more accurately—we can calculate the shift in eigenvalues using converged Dirac wave
functions in response to the combined effect of the Coulomb and vacuum polarization potentials. In this case we simply take the difference between the converged eigenvalues for the $2S_{1/2}$ and $2P_{1/2}$ eigenstates calculated in the presence of point-Coulomb and point-vacuum polarization potentials

$$\Delta E^{2S-2P}_{\text{Lamb}} = \lambda_{2P_{1/2}} - \lambda_{2S_{1/2}} = 205.1706(5) \text{ meV},$$  \quad (14)

Care must be taken when comparing this calculation to that of Eq. (13) since our calculation includes relativistic corrections, which are treated as corrections to Eq. (13) in Ref. [1]. A summary of this comparison and the calculated values for the Lamb shift are given in Table II where we note that the perturbative and non-perturbative calculations are found to be in good agreement. For this table and those that follow, we refer to various iterations of our calculations in which we compute the wave function in the presence of point-Coulomb (C); finite (size nucleus)-Coulomb (FC); point vacuum polarization (VP); and finite (size nucleus) vacuum polarization (FVP) potentials. The dependence on the finite size of the proton arises from considerations of charge-distribution—whether it be exponential, Yukawa, or Gaussian in form—appears to be extremely weak.

The exponential form for the charge-distribution, normalised to unity such that $\int \rho(r) \, d^3r = 1$ is given by

$$\rho(r) = \frac{\eta}{8\pi} e^{-\eta r}; \quad \eta = \sqrt{12/(r_p^2)}.$$  \quad (17)

We calculate the Lamb shift by taking the difference between the appropriate eigenvalues calculated using the Dirac equation with the potential given by Eq. (16) with the charge-distribution given by Eq. (17) for various values of $\langle r_p^2 \rangle$. We then interpolate the energy shifts and fit the data to a cubic of the form

$$f(x) = A(r_p^2) + B(r_p^2)^{3/2},$$  \quad (18)

which provides the relevant parameterization. The $\langle r_p^2 \rangle^n$ dependence in the presence of an exponential finite-sized Coulomb potential and point vacuum polarization potential

$$V(r) = -Z\alpha \int \frac{\rho(r')}{|r - r'|} \, d^3r' + V_{\text{VP}}(r),$$  \quad (19)

given by

$$\Delta E_{\text{Finite}} = 205.1706 - 5.2169 \langle r_p^2 \rangle + 0.0353 \langle r_p^2 \rangle^{3/2} \text{ meV},$$  \quad (20)

A further important effect of the finite size of the proton arises through the convolution of the vacuum polarization potential (Eq. (12)) with the proton charge-distribution. This leads to the replacement of the point vacuum polarization potential by

$$V_{\text{VP}}(r) \to \frac{-2Z\alpha^2}{3\pi} \int \frac{\rho(r')}{|r - r'|^3} Z_0(|r - r'|) \, dr',$$

where we use the expression given in Ref. [11]

$$Z_n(|r'|) = \int_1^{\infty} e^{-\frac{2}{\lambda} d|\xi|} \left(1 + \frac{1}{2\xi^2}\right) \frac{\xi^2 - 1}{\xi^2} \, d\xi,$$

and where $\lambda$ denotes the electron Compton wavelength (divided by $2\pi$), $\lambda = 386.15926459 \text{ fm}$. When discussing this potential, it should be assumed that we are using a normalised exponential charge-distribution. We once again calculate the eigenvalues using various values of $\langle r_p^2 \rangle$ in the charge-distribution and fit the resulting energies to a cubic (as per Eq. (13)), except that in this case the vacuum polarization induces the Lamb shift, and we must include a term proportional to 1. Thus we find

$$\Delta E_{\text{Finite}} = 205.182 - 5.2519 \langle r_p^2 \rangle + 0.0546 \langle r_p^2 \rangle^{3/2} \text{ meV},$$  \quad (23)
TABLE I: Contributions to the 2S–2P Lamb shift with comparison to values presented in Pohl et al.\cite{7} which themselves are selected values from various theoretical sources—references 1–5, 11, 12, 14–17, and 19–25 of Pohl et al.. Values are all in meV. Errors in the Dirac calculations are taken to be ±500 meV as per Section IIIV. We refer to various iterations of our calculations in which we compute the wave function in the presence of point-Coulomb (C); finite-Coulomb (FC); point vacuum polarization (VP); and finite vacuum polarization (FVP) potentials. The dependence on \(r^2\) is extracted in each case by fitting the energy shifts calculated at various values of \(r\) to a cubic of the form given in Eq. (18) for the case of a Coulomb-only potential, and with the addition of a term proportional to 1 when including the vacuum polarization. The listed corrections are already included in our Dirac calculations, namely lines 3 and 5 of Table 1 in Ref. [7] and the nuclear size contributions of Table 2 from that reference. All further corrections to both the perturbative calculation and our calculation are contained in ‘Remaining Corrections’ which in this case encompasses all remaining contributions of Table 1 and radiative correction of Table 2 of Ref. [7].

| Contribution | Pohl et al. | Present Work |
|--------------|------------|--------------|
| Dirac \((V = V_C + V_{VP})\) | | 205.1706 |
| Dirac \((V = V_{FC})\) | -5.2000 \(\langle r_p^2 \rangle\) + 0.0350 \(\langle r_p^2 \rangle^{3/2}\) | | |
| Dirac \((V = V_{FC} + V_{VP})\) | 205.1706 - 5.2169 \(\langle r_p^2 \rangle\) + 0.0353 \(\langle r_p^2 \rangle^{3/2}\) | | |
| Dirac \((V = V_{FC} + V_{PVP})\) | 205.1822 - 5.2519 \(\langle r_p^2 \rangle\) + 0.0546 \(\langle r_p^2 \rangle^{3/2}\) | | |
| Relativistic one loop VP | 205.0282 | | |
| Polarization insertion in two Coulomb lines | | 0.1509 |
| Finite size effects | -5.1987 \(\langle r_p^2 \rangle\) + 0.0347 \(\langle r_p^2 \rangle^{3/2}\) | | |
| Subtotal: | 205.1791 - 5.1987 \(\langle r_p^2 \rangle\) + 0.0347 \(\langle r_p^2 \rangle^{3/2}\) | 205.1822 - 5.2519 \(\langle r_p^2 \rangle\) + 0.0546 \(\langle r_p^2 \rangle^{3/2}\) |
| Remaining Corrections | 0.8782 - 0.0275 \(\langle r_p^2 \rangle\) | | |
| Total: | 206.0573 - 5.2262 \(\langle r_p^2 \rangle\) + 0.0347 \(\langle r_p^2 \rangle^{3/2}\) | 206.0604 - 5.2794 \(\langle r_p^2 \rangle\) + 0.0546 \(\langle r_p^2 \rangle^{3/2}\) |

which is the expression which is compared to the perturbative calculation in Table II. We note that the finite-vacuum polarization induces a small but non-trivial shift, and that the results are otherwise essentially the same as those of Pohl et al.\cite{7}.

VII. 2P FINE STRUCTURE

The \(O(\alpha^4)\) perturbative 2P fine structure splitting is calculated in Ref.\cite{3} to be

\[
\Delta E_{FS}^{2P} = \frac{\mu^3 (Z\alpha)^4}{32m^2_p} \left(1 + \frac{2m_\mu}{m_p}\right),
\]

along with higher-order corrections. Taking this splitting as the difference between the converged eigenvalues of the 2P\(_{1/2}\) and 2P\(_{3/2}\) eigenstates gives

\[
\Delta E_{FS}^{2P} = \lambda_{2P_{3/2}} - \lambda_{2P_{1/2}},
\]

which we can also calculate in the presence of the various potentials. For the case of an exponential finite-Coulomb potential with finite vacuum polarization, the 2P fine structure splitting is

\[
\Delta E_{FS}^{2P} = 8.4206(5) \text{ meV}.
\]

A comparison of this value with perturbative calculations of Boric\cite{1} is presented in Table III. The effect of the finite-size Coulomb potential (as compared to the point case) is negligible at the level of errors of our calculation. Similarly, the effect of the finite-size vacuum polarization is also negligible at our level of errors. The vacuum polarization itself increases the fine structure splitting by 5 µeV. We note that the perturbative and non-perturbative calculations are in perfect agreement to the level of errors presented here.

VIII. HYPERFINE STRUCTURE

The hyperfine structure is a measure of the \(\vec{l} \cdot \vec{\sigma}\) coupling. Following the lead of Ref.\cite{21}, the appropriate Hamiltonian is given by

\[
\mathcal{H} = 2\beta_\mu \gamma \hbar \ell (\ell + 1) \frac{1}{j(j+1)} I \cdot J + \frac{16\pi}{3} \beta \gamma \hbar |\psi(0)|^2 I \cdot S,
\]

comprising a dipole term and a contact term, for which the following definitions apply for the muon Bohr magneton \(\beta_\mu\); proton Bohr magneton \(\beta_p\); and proton gyromagnetic ratio \(\gamma\)

\[
\beta_\mu = \sqrt{\alpha}/2m_\mu, \quad \beta_p = \sqrt{\alpha}/2M_p, \quad \gamma = 2(1 + \kappa)\beta_p.
\]

Here \(\kappa = 1.792847351\) is the proton anomalous magnetic moment. \(|\psi(0)|^2\) represents the muon wave function at the
TABLE II: Contributions to the 2P fine-structure splitting with comparison to values found in Borie [1]. Subscripts are defined in Table I. Values are all in meV. Errors in the Dirac calculations are taken to be ±500 neV as per Section IV. The listed correction (Uehling/vacuum polarization) is already included in our Dirac calculations. All further corrections to both the perturbative calculation and our calculation are contained in ‘Remaining Corrections’ which are detailed in Table II of Ref. [1].Finite-size effects in either the Coulomb or vacuum polarization potentials provide no shift above the level of errors here, as expected for P-states. The perturbative calculation prediction is reproduced within errors.

| Contribution | Borie | Present Work |
|--------------|-------|--------------|
| Dirac (V = VC) | 8.4156 | 8.4156 |
| Dirac (V = VF) | 8.4156 | 8.4156 |
| Dirac (V = VC + VVP) | 8.4206 | |
| Dirac (V = VF + VVP) | 8.4206 | |
| Dirac (V = VPC + VVP) | 8.4206 | |
| Uehling (VP) | 0.0050 | |
| Subtotal | 8.4206 | 8.4206 |
| Remaining Corrections | -0.06852 | |
| Total | 8.3521 | 8.3521 |

We now investigate the two terms of Eq. (27) separately.

A. 2S\textsubscript{1/2} Hyperfine Structure

There exist several methods by which the 2S hyperfine structure can be calculated. The perturbative 2S hyperfine structure calculated in Ref. [4] is given by

\[ \Delta E_{\text{2S}_{\text{HF}}F} = \frac{1}{3}(Za)^4 \frac{\hbar^2}{m_p \mu_p} (1 + \kappa). \] (29)

For \( \ell = 0 \) the contact term in the Hamiltonian (Eq. (27)) is non-zero, while the dipole term vanishes;

\[ E_{\text{2S}_{\text{HF}}F} = \frac{16\pi}{3} \beta \gamma h |\psi(0)|^2 \langle Fm_F|\mathbf{I}\cdot\mathbf{S}|Fm_F \rangle, \] (30)

where \( |Fm_F \rangle \) is the eigenfunction belonging to \( \mathbf{F} = \mathbf{I} + \mathbf{J} \), such that

\[ \langle Fm_F|\mathbf{I}\cdot\mathbf{S}|Fm_F \rangle = \frac{1}{2} \left[ F(F + 1) - \frac{3}{2} \right]. \] (31)

Thus, the splitting between the 2\textsubscript{S} \( F = 0 \) and \( F = 1 \) hyperfine levels is given by

\[ \Delta E_{\text{2S}_{\text{HF}}F} = \frac{16\pi}{3} \beta \gamma h |\psi(0)|^2, \] (32)

We note an important, relevant typographical correction; In Ref. [21], Eq. (18.2-17b), the sign should be positive and the second 9 in the denominator should not appear.

The value of the 2\textsubscript{S} hyperfine splitting, as calculated using Eq. (32) with the wave function calculated with the Dirac equation in the presence of the combined exponential finite-Coulomb and finite vacuum polarization potentials is

\[ \Delta E_{\text{2S}_{\text{HF}}F} = 22.7690(5) \text{ meV}. \] (33)

We note that the effect of including the exponential finite-size Coulomb potential as compared to the point case reduces the splitting by 0.1269(5) meV; introducing the point vacuum polarization potential increases the splitting by 0.0747(5) meV for the point-Coulomb, and 0.0742(5) meV for the finite-Coulomb cases. Using the combined finite vacuum polarization and finite-Coulomb potentials reduces the splitting by 0.0012(5) meV to give the value above.

Alternatively, one can follow Ref. [2] in which case we can calculate this splitting to be

\[ \Delta E_{\text{2S}_{\text{HF}}F} = \frac{k^2}{\kappa^2 - \frac{1}{4}} \left[ \Lambda(\Lambda + 1) - I(I + 1) - j(j + 1) \right] \]
\[ \times \frac{\alpha}{2\kappa^2} \int r^{-2} g(r) f(r) dr. \] (34)

In that case, we calculate

\[ \Delta E_{\text{2S}_{\text{HF}}F} = 22.7640(5) \text{ meV}, \] (35)

provided we correct for the reduced mass in the formula such that the magnetic moment of the muon is not defined in terms of reduced mass but rather defined in terms of the free space mass.

A comparison to perturbative calculations is given in Table III where we note the finding of a finite-size dependent contribution in this splitting, which is neglected in the summary of Pohl et al. (though finite-size effects sans a parameterization are calculated in studies by Borie [1] and Pachucki [3]) and which differs from results obtained using the standard Zemach treatment [2]. We note that for \( \langle \gamma^2 \rangle_\mu = 0.8768 \text{ fm} \), the 2\textsubscript{S}\textsubscript{1/2} hyperfine splitting is calculated here to be 22.8496 meV (22.8547 meV for \( \langle \gamma^2 \rangle_\mu = 0.84184 \text{ fm} \) which indicates a 0.0087(5) meV (0.0100(5) meV) correction to the perturbative calculation (once the factor of 1/4 is taken into account), or 2.8–3.2% of the 0.31 meV quoted discrepancy.

B. 2P\textsubscript{1/2} Hyperfine Structure

The 2\textsubscript{P}\textsubscript{1/2} hyperfine structure is of no consequence for the transition which we are investigating here. Nonetheless, we calculate the energy of the 2\textsubscript{P}\textsubscript{1/2} = 0 and 2\textsubscript{P}\textsubscript{1/2} = 1 levels as a confirmation of our method, and to compare to the perturbative results. Following Ref. [2], to \( \mathcal{O}(\alpha^4) \) the 2\textsubscript{P}\textsubscript{1/2} hyperfine structure splitting is given by

\[ \Delta E_{\text{2P}_{\text{HF}}F} = E_F \left[ \frac{1}{3} + \frac{\alpha}{6} + \frac{m_p(1 + 2\kappa)}{12m_p(1 + \kappa)} \right]. \] (36)
TABLE III: Contributions to the $2S_{1/2}$ hyperfine splitting calculated via Eq. (32) with comparison to values found in Martynenko [4]. Subscripts are defined in Table [I]. Values are all in meV. Errors in the Dirac calculations are taken to be ±500 neV as per Section [IV]. 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 'Proton structure corrections of $O(\alpha^5)$' pertains to the Zemach contribution (which we shall explore in an upcoming publication) and does not include considerations of finite-size in the wavefunction, and that the polynomial dependence on $\langle r_p^2 \rangle^n$ of this splitting is not discussed in the literature.

| 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 $\frac{\hbar^2}{m}(Z\alpha)^2 E_F$ | 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   |              |
| Subtotal:                              | 22.7291    | 22.8521 - 0.1795 (\langle r_p^2 \rangle + 0.0739 (\langle r_p^2 \rangle^{3/2})] |
| Remaining Corrections                 | 0.0857     |              |
| Total:                                | 22.8148    | 22.9378 - 0.1795 (\langle r_p^2 \rangle + 0.0739 (\langle r_p^2 \rangle^{3/2})] |
for which the Fermi energy is

\[ E_F = \frac{\mu^3(1 + \kappa)}{3m_pm_p} (Z\alpha)^4, \tag{37} \]

and where \( \alpha_n \) is the muon anomalous magnetic moment. We note another important, relevant typographical correction; in Ref. [3] the factors of 2 in the denominators of the third terms of Eqs. (27–28) should read 12. The calculations are performed correctly however. For \( \ell \neq 0 \), the dipole term in the Hamiltonian (Eq. (27)) is non-zero, while the contact term vanishes. The energy for the dipole term is thus given by

\[ E_{HFS}^{2P_{1/2}} = 2\beta\gamma \hbar \frac{\ell(\ell + 1)}{j(j+1)} \frac{1}{r^3} \langle Fm_F | I \cdot J | Fm_F \rangle, \tag{38} \]

where the non-zero terms in the dot-product are given by

\[ \langle Fm_F | I \cdot J | Fm_F \rangle = \frac{1}{2} [F(F+1) - I(I+1) - j(j+1)]. \tag{39} \]

For Schrödinger wave functions, the vacuum expectation value of \( r^{-3} \) is analytic, in that

\[ \langle 1/r^3 \rangle = \left( a_0^3 n^3 \ell(\ell + 1)(\ell + 1/2) \right)^{-1}. \tag{40} \]

Inserting the appropriate values of \( F, n, \ell, I, j \) for each of the \( F = 0 \) and \( F = 1 \) states, one obtains the energy of the \( 2P_{1/2} \) hyperfine structure to be

\[ \Delta E_{HFS}^{2P_{1/2}} = \frac{2}{9} \beta\gamma \hbar / a_0^3. \tag{41} \]

Eq. (41) corresponds to the leading term of Eq. (36), to which the anomalous magnetic moments provide additional corrections. Using the converged Dirac wave functions with exponential finite-Coulomb and finite vacuum polarization potentials (rather than Schrödinger wave functions) we calculate the expectation value of \( r^{-3} \) and find

\[ \Delta E_{HFS}^{2P_{1/2}} = 7.6204(5) \text{ meV}. \tag{42} \]

The results of this calculation are summarised in Table IV, where we note that the addition of the (point) vacuum polarization potential to the point-Coulomb potential increases the splitting by 0.0017(5) meV, and the introduction of the finite-Coulomb potential increases this further by 0.0045(5) meV to arrive at the value above. The effect of finite-vacuum polarization is essentially zero here.

### C. \( 2P_{3/2} \) Hyperfine Structure

Following the same method as in the previous subsection, we can calculate the energy levels for the \( 2P_{3/2} \) and

| Contribution          | Martynenko | Present Work |
|-----------------------|------------|--------------|
| Dirac \((V = V_C)\)   | 7.6141     | 7.6159       |
| Dirac \((V = V_C + V_{VP})\) | 7.6204     |              |
| Dirac \((V = V_{FC} + V_{VP})\) | 7.6204     |              |
| Leading contribution  | 7.6018     |              |
| \(\mathcal{O}(Z\alpha)^6\) contribution | 0.0011     |              |
| Subtotal              | 7.6029     | 7.6204       |
| Remaining Corrections | 0.3615     |              |
| Total                 | 7.9644     | 7.9819       |

The results of this calculation are summarised in Table IV, where we note that the addition of the (point) vacuum polarization potential to the point-Coulomb potential increases the splitting by 0.0017(5) meV, and the introduction of the finite-Coulomb potential increases this further by 0.0045(5) meV to arrive at the value above. The effect of finite-vacuum polarization is essentially zero here.

\[ \Delta E_{HFS}^{2P_{3/2}} = 3.0415(5) \text{ meV} \tag{44} \]

when the potential consists of the exponential finite-Coulomb and point vacuum polarization potentials. For this state, the addition of the (point) vacuum polarization potential to the point-Coulomb potential increases the splitting by 0.0007(5) meV to the value listed in Table IV, and the introduction of the finite-Coulomb potential was found to have no effect within the limits of our calculation, so too was the introduction of the finite vacuum polarization potential.
TABLE V: Contributions to the $2P_{3/2}$ hyperfine splitting with comparison to values found in Martynenko [5]. Subscripts are defined in Table IV. Values are all in meV. Errors in the Dirac calculations are taken to be ±500 neV as per Section IV

| Contribution | Martynenko | Present Work |
|--------------|------------|--------------|
| Dirac ($V = V_{C}$) | 3.0408 | |
| Dirac ($V = V_{C} + V_{F}$) | 3.0415 | |
| Dirac ($V = V_{FC} + V_{VP}$) | 3.0415 | |
| Dirac ($V = V_{FC} + V_{VP}$) | 3.0415 | |
| Leading contribution | 3.0407 | |
| Relativistic correction | 0.0001 | |
| Subtotal | 3.0408 | 3.0415 |
| Remaining Corrections | 0.3518 | |
| Total: | 3.3926 | 3.3933 |

IX. SUMMARY

We summarise the findings of these non-perturbative Dirac calculations and compare to the previous literature values of perturbative calculations in Table VI. We add to this a combined expression for the cubic which when set equal to the experimental value of the measured transition is solved to predict the proton rms charge-radius, as is done in Ref. [7].

We do not include the result of hyperfine splitting calculations for the $2P_{1/2}$ eigenstate as this is of no relevance to the measured transition. We also note the omission here of the energy shift attributed to a mixing between the $2P_{1/2}$ and $2P_{3/2} F = 1$ states, as discussed in Ref. [6] for comparison to Ref. [7] where it is also absent.

We find that the perturbative calculations are largely reproduced using our methods when considering the appropriate potentials for comparison. We further find that in several cases the use of the finite-vacuum polarization potential produces effects which are not accounted for in previous studies. The largest of these is the finite-size contribution to the $2S_{1/2}$ hyperfine splitting which has been neglected in the literature up to this point.

Overall, the non-perturbative calculations do not elucidate any missing contributions of a magnitude large enough to resolve the proton radius problem outlined in Pohl et al. [7].

X. CONCLUSIONS

After careful consideration of the various contributions to the measured transition energy of Pohl et al. [7], calculated consistently using the Dirac equation with appropriate potentials, and following the addition of the required corrections to these calculations (taking further care to avoid overcounting issues), we find no single term which leads to a discrepancy with the perturbative results of sufficient magnitude to account for the discrepancy reported in Ref. [7]. These calculations nonetheless provide a useful insight into the reliability of the perturbative calculations, and allow a simpler approach to future investigations.

While it remains possible in principle that one or more of the higher-order corrections to the terms calculated in this work might be of sufficient magnitude to affect the analysis of Ref. [7], the precision with which the Dirac and perturbative calculations agree for the terms which we have calculated here strongly suggests that this will not be the case.

In addition to the calculations presented here, we further note that our calculations of a hitherto overlooked contribution arising from off-mass-shell effects for the proton (which are negligible for electronic hydrogen) provide a natural solution to the proton radius problem [12], and as such the combination of these two sets of calculations may be seen as a complete description of the measured transition in muonic hydrogen with no discrepancy in the rms charge radius of the proton. Because of the uncertain magnitude of the off-mass-shell effects, it is incorrect to complete the analysis of this transition to predict a proton rms charge radius—we await the results of current and future experiments which will be ascertain the strength of this contribution, after which a complete analysis will be possible.

Nonetheless, we note that our calculations predict that the transition energy for the $2P_{3/2}^{F=2}$ to $2S_{1/2}^{F=1}$ transition in muonic hydrogen is larger in magnitude than that which is predicted by the perturbative calculations, and that analysis of this data under the assumption that no further terms are required leads to the following values for the proton rms charge radius when fit to the experimental data:

\[
\text{Pohl et al.: } \sqrt{\langle r_p^2 \rangle} = 0.84183(67) \text{ fm,}
\]

\[
\text{Present Work: } \sqrt{\langle r_p^2 \rangle} = 0.83811(67) \text{ fm.}
\]

The value listed as Present Work is taken as the solution to the cubic equation

\[209.9505 - 5.2345\langle r_p^2 \rangle + 0.0361\langle r_p^2 \rangle^{3/2} = 206.2949, \quad (45)\]

where the right-hand-side corresponds to the quoted value of the measured transition in Ref. [7]; the left-hand-side is taken from the relevant conclusion line of Table IV and for which the errors in this calculation are dominated by the experimental error. The extracted $\sqrt{\langle r_p^2 \rangle}$ value listed as Pohl et al. is taken from Ref. [7] (calculated in the same fashion) and differs from the central value...
TABLE VI: Sum of perturbative and non-perturbative theoretical contributions to the measured experimental transition energy shown in Fig. 1. Subscripts are defined in Table I. Values are all in meV. The individual perturbative contributions (listed under ‘Various’) are taken from Tables II–V. In each case, the value given for the Dirac calculation is calculated using the combination of finite-Coulomb and finite vacuum polarization potentials ($V = V_{FC} + V_{FVP}$). The fractional factors for the hyperfine splittings are inserted for relevance to the measured transition, and are calculated via angular-momentum splitting rules.

| Contribution                        | Various  | Present Work |
|-------------------------------------|----------|--------------|
| $2S_{1/2}$-$2P_{1/2}$ Lamb shift (constant) | 206.0573 | 206.6004     |
| $2S_{1/2}$-$2P_{1/2}$ Lamb shift (finite-size) | -5.2620($r_p^2$) + 0.0347($r_p^2$)/3/2 -5.2794($r_p^2$) + 0.0546($r_p^2$)/3/2 |
| $2P$ Fine Structure                 | 8.3521   | 8.3521       |
| $\frac{1}{2} \times 2S_{1/2}$ Hyperfine (constant) | -5.7037  | -5.7345      |
| $\frac{1}{2} \times 2S_{1/2}$ Hyperfine (finite-size) | 0.0000   | 0.0449 ($r_p^2$) - 0.0185 ($r_p^2$)/3/2 |
| $\frac{1}{2} \times 2P_{3/2}$ Hyperfine   | 1.2722   | 1.2725       |
| (Various) Total (Perturbative)       | 209.9779 - 5.2262 ($r_p^2$) + 0.0347 ($r_p^2$)/3/2 |
| (Present Work) Total (Dirac)         | 209.9505 - 5.2345 ($r_p^2$) + 0.0361 ($r_p^2$)/3/2 |
quoted in [7]; $0.84184(67)$, though the difference is well within the quoted errors.

We note the degree to which the cubic expression Eq. (45) agrees with that of Ref. [7], despite the latter not involving a calculation of a finite-size contribution to the $2S$ hyperfine splitting. Some research in progress by the authors will elucidate some further overlooked contributions that will likely alter the agreement between these two expressions, and we look forward to future measurements with which we may compare our findings.

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