Model Independent Analysis of Proton Structure for Hydrogenic Bound States

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Proton structure effects in hydrogenic bound states are analyzed using nonrelativistic QED effective field theory. Implications for the Lamb shift in muonic hydrogen are discussed. Model-dependent assumptions in previous analyses are isolated, and sensitivity to poorly constrained hadronic structure in the two-photon exchange contribution is identified.

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Introduction.—Atomic spectroscopy can provide the most precise determination of fundamental hadron properties, such as the proton radius [1–3]. The need for systematic analysis to translate between bound state energies and hadronic observables is sharpened by a discrepancy between the recent muonic hydrogen Lamb shift measurement [2] and existing theoretical calculations. Using a model-independent extraction of the charge radius from electron scattering data ($r = 0.871(10)$ fm [4]; see also [5,6]) or an extraction from electronic hydrogen spectroscopy ($r = 0.8768(69)$ fm [3]; see also [7]), the measured $2S^{(F=1)}_{j=1/2} - 2P^{(F=2)}_{j=3/2}$ interval in muonic hydrogen lies 0.258 (90) meV or 0.311(63) meV above theory. The discrepancy brings into question the treatment of proton structure effects in atomic bound states, and has generated speculations on new forces acting in the muon-proton system [8], inadequate treatment of proton charge density correlations [9], and modifications of off-shell photon vertices [10].

Nonrelativistic QED (NRQED) [11] is a field theory describing the interactions of photons and nonrelativistic matter. The NRQED Lagrangian is constructed to yield predictions valid to any fixed order in small parameters α and $|\boldsymbol{q}|/M$, where $|\boldsymbol{q}|$ denotes a typical bound state momentum, and M is a mass scale for the nonrelativistic particle. NRQED provides a rigorous framework to study the effects of proton structure, avoiding problems of double counting in bound state energy computations [12], eliminating difficulties of interpretation for the polarizability of a strongly interacting particle [13], and providing trivial derivations of universal properties, such as the low energy theorems of Compton scattering [14].

We examine the NRQED framework for determining proton structure corrections in atomic bound states. The Lamb shift in muonic hydrogen is the first measurement directly sensitive to the spin-independent, proton structure-dependent, contact interaction appearing in NRQED (d_2 below). The strength of this interaction is not determined by measured on-shell form factors, or inelastic structure functions of the proton. We identify model-dependent assumptions in previous analyses and discuss whether poorly constrained proton structure corrections can account for the above-mentioned discrepancy. We conclude by outlining extensions of the theoretical analysis and related applications.

NRQED.—Consider the formalism for electron-proton bound states; the substitution $e \to \mu$ applies for the muon-proton system. The NRQED Lagrangian can be decomposed as $\mathcal{L}_{\rm NRQED} = \mathcal{L}_\gamma + \mathcal{L}_e + \mathcal{L}_p + \mathcal{L}_{\rm contact}$. $\mathcal{L}_\gamma$ contains the photon kinetic term and vacuum polarization corrections; these corrections can be treated separately and will not be considered here. Through $\mathcal{O}(1/m_e^3)$, [11,15,16]

$$\mathcal{L}_e = \psi_e^\dagger \Big\{ iD_t + \frac{\boldsymbol{D}^2}{2m_e} + \frac{\boldsymbol{D}^4}{8m_e^3} + c_F e \frac{\boldsymbol{\sigma}\cdot\boldsymbol{B}}{2m_e} + c_D e \frac{[\boldsymbol{\partial}\cdot\boldsymbol{E}]}{8m_e^2} + i c_S e \frac{\boldsymbol{\sigma}\cdot(\boldsymbol{D}\times\boldsymbol{E} - \boldsymbol{E}\times\boldsymbol{D})}{8m_e^2} + c_{W1} e \frac{\{\boldsymbol{D}^2, \boldsymbol{\sigma}\cdot\boldsymbol{B}\}}{8m_e^3} - c_{W2} e \frac{D^i \boldsymbol{\sigma}\cdot\boldsymbol{B} D^i}{4m_e^3} + c_{p'p} e \frac{\boldsymbol{\sigma}\cdot\boldsymbol{D}\boldsymbol{B}\cdot\boldsymbol{D} + \boldsymbol{D}\cdot\boldsymbol{B}\boldsymbol{\sigma}\cdot\boldsymbol{D}}{8m_e^3} + i c_M e \frac{\{D^i, [\boldsymbol{\partial}\times\boldsymbol{B}]^i\}}{8m_e^3} + c_{A1} e^2 \frac{\boldsymbol{B}^2 - \boldsymbol{E}^2}{8m_e^3} - c_{A2} e^2 \frac{\boldsymbol{E}^2}{16 m_e^3} \Big\} \psi_e . \tag{1}$$

Here ψ_e is a two-component spinor representing the nonrelativistic electron field, $\boldsymbol{\sigma}$ is the Pauli spin matrix, D_t and $\boldsymbol{D}$ are covariant derivatives and $\boldsymbol{E}$, $\boldsymbol{B}$ are the electric and magnetic fields. Prefactors are chosen for convenience so that for a pointlike fermion at tree level, $c_F = c_D = c_S = c_{W1} = c_{A1} = 1$ and $c_{W2} = c_{p'p} = c_M = c_{A2} = 0$.

A similar expression holds for $\mathcal{L}_p$ with $e \to -Ze$ ($Z = 1$ for the proton). Relevant contact interactions in the single proton plus single electron sector are

$$\mathcal{L}_{\rm contact} = d_1 \frac{\psi_p^\dagger \boldsymbol{\sigma}\psi_p \cdot \psi_e^\dagger \boldsymbol{\sigma}\psi_e}{m_e m_p} + d_2 \frac{\psi_p^\dagger \psi_p \psi_e^\dagger \psi_e}{m_e m_p} . \tag{2}$$

The coefficients c_i, d_i depend on the choice of ultraviolet regulator. Since no new bound state computations are necessary, we will quote results for phenomenological inputs and bound state energies that are independent of this choice. We are interested in proton structure corrections to energy levels through order $m_e^3\alpha^5/m_p^2$, and therefore need $c_{F,D,S}$ in $\mathcal{L}_p$ through $\mathcal{O}(\alpha)$, and $d_{1,2}$ through $\mathcal{O}(\alpha^2)$. Other operators in $\mathcal{L}_p$ will enter when we analyze the low Q^2 expansion of the forward Compton amplitude to constrain d_2. Knowledge of the c_i's and d_i's allows us to determine corrections to energy levels. For example, coefficients c_D^{proton} and d_2 lead to first order energy shifts

$$\delta E(n,\ell) = \delta_{\ell 0}\frac{m_r^3(Z\alpha)^3}{\pi n^3}\left(\frac{Z\alpha\pi}{2m_p^2}c_D^{\text{proton}} - \frac{1}{m_e m_p}d_2\right), \quad (3)$$

where $m_r = m_e m_p/(m_e + m_p)$ is the reduced mass.

Matching.—The NRQED Wilson coefficients are determined by enforcing matching conditions between full and effective theories using convenient low energy observables. We concentrate on the matching conditions for the proton.

One photon matching.—Wilson coefficients for operators coupling to a single photon are determined in terms of the proton elastic form factors and their derivatives at $q^2 = 0$ by using (1) to compute the amplitude for elastic scattering of a proton via the electromagnetic current [16–18]. The form factors satisfy $F_1(0) = 1$, $F_2(0) = a_p$,

$$\begin{aligned} F_1'(0) &= \frac{1}{6}(r_E^p)^2 - \frac{a_p}{4m_p^2} + \frac{Z^2\alpha}{3\pi m_p^2}\log\frac{m_p}{\lambda}, \\ F_2'(0) &= \frac{1}{6}[(1+a_p)(r_M^p)^2 - (r_E^p)^2] + \frac{a_p}{4m_p^2}, \end{aligned} \quad (4)$$

where λ is a photon mass [19]. These expressions serve to define the phenomenological parameters $a_p \approx 1.793$, r_E^p, and r_M^p.

Two-photon matching.—The coefficients c_{A1}, c_{A2} can be determined by comparing to spin-averaged amplitudes for forward and backward Compton scattering in the lab frame [17]

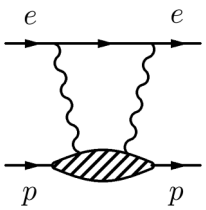

FIG. 1. Two-photon exchange amplitude for $e^- p \to e^- p$ scattering.

$$\begin{aligned} 4m_p^3\bar{\alpha}/\alpha &= -c_{A1} - c_{A2}/2 + 1 + 2c_M + c_F c_S - c_F^2, \\ 4m_p^3\bar{\beta}/\alpha &= c_{A1} - 1, \end{aligned} \quad (5)$$

where $\bar{\alpha} = 12.0(6)\times 10^{-4}$ fm^3 and $\bar{\beta} = 1.9(5)\times 10^{-4}$ fm^3 [20].

Contact interactions.—The coefficients in (2) can be fixed using the zero-momentum limit for $e^- p \to e^- p$ scattering, cf. Fig. 1. The tree level, $\mathcal{O}(\alpha)$, amplitude is reproduced by the effective field theory, and the d_i's receive a nonzero contribution starting at $\mathcal{O}(\alpha^2)$. We focus on the spin-independent case and neglect higher order radiative corrections. The relevant proton matrix element is the forward Compton amplitude ($\nu = 2k\cdot q$, $Q^2 = -q^2$)

$$\begin{aligned} &\frac{1}{2}\sum_s i\int d^4x e^{iq\cdot x}\langle \boldsymbol{k}, s|T\{J^\mu_{\text{e.m.}}(x)J^\nu_{\text{e.m.}}(0)\}|\boldsymbol{k}, s\rangle \\ &\quad = (-g^{\mu\nu} + q^\mu q^\nu/q^2)W_1(\nu, Q^2) \\ &\qquad + (k^\mu - k\cdot q q^\mu/q^2)(k^\nu - k\cdot q q^\nu/q^2)W_2(\nu, Q^2). \end{aligned} \quad (6)$$

Our normalizations are such that for a point particle, $W_1 = 2\nu^2/(Q^4 - \nu^2)$ and $W_2 = 8Q^2/(Q^4 - \nu^2)$. The matching condition for the spin-averaged zero-momentum four-point amplitude is

$$\begin{aligned} &\frac{4\pi m_r}{\lambda^3} - \frac{\pi m_r}{2m_e m_p\lambda} - \frac{2\pi m_r}{m_p^2\lambda}[F_2(0) + 4m_p^2 F_1'(0)] - \frac{2}{m_e m_p}\left[\frac{2}{3} + \frac{1}{m_p^2 - m_e^2}\left(m_e^2\log\frac{m_p}{\lambda} - m_p^2\log\frac{m_e}{\lambda}\right)\right] + \frac{\delta d_2 (Z\alpha)^{-2}}{m_e m_p} \\ &\quad = -\frac{m_e}{m_p}\int_{-1}^{1} dx\sqrt{1-x^2}\int_0^\infty dQ\,\frac{Q^3[(1+2x^2)W_1(2im_p Qx, Q^2) - (1-x^2)m_p^2 W_2(2im_p Qx, Q^2)]}{(Q^2+\lambda^2)^2(Q^2+4m_e^2x^2)}, \end{aligned} \quad (7)$$

where δd_2 denotes the contribution to d_2 in addition to the point-particle value.

The imaginary part of the W_i's can be related to measured quantities. By inserting a complete set of states into (6), the proton contribution to $\text{Im}W_i$ is expressed in terms of proton form factors, and the continuum contribution to $\text{Im}W_i$ is determined by inelastic structure functions. Using dispersion relations, W_2 can be fully reconstructed from its imaginary part. Since W_1 requires a subtraction for a convergent dispersion relation, knowledge of $W_1(0, Q^2)$ is also needed. Thus W_i can be written

$$\begin{aligned} W_1(\nu, Q^2) &= W_1(0, Q^2) + W_1^{p,1}(\nu, Q^2) + W_1^{c,1}(\nu, Q^2), \\ W_2(\nu, Q^2) &= W_2^{p,0}(\nu, Q^2) + W_2^{c,0}(\nu, Q^2), \end{aligned} \quad (8)$$

where the superscript numbers denote the number of subtractions. The proton terms are

$$W_1^{p,1}(\nu, Q^2) = 2\nu^2(F_1 + F_2)^2/(Q^4 - \nu^2),$$
$$W_2^{p,0}(\nu, Q^2) = 2Q^2(4F_1^2 + Q^2F_2^2/m_p^2)/(Q^4 - \nu^2), \quad (9)$$

with $F_i \equiv F_i(-Q^2)$. The continuum terms are

$$W_1^{c,1}(\nu, Q^2) = \frac{\nu^2}{\pi}\int_{\nu_{\rm cut}(Q^2)^2}^{\infty} d\nu'^2 \frac{{\rm Im}W_1(\nu', Q^2)}{\nu'^2(\nu'^2 - \nu^2)},$$
$$W_2^{c,0}(\nu, Q^2) = \frac{1}{\pi}\int_{\nu_{\rm cut}(Q^2)^2}^{\infty} d\nu'^2 \frac{{\rm Im}W_2(\nu', Q^2)}{\nu'^2 - \nu^2}, \quad (10)$$

where $\nu_{\rm cut}(Q^2) = Q^2 + 2m_\pi m_p + m_\pi^2$ is the threshold for pion production, and ${\rm Im}W_i(\nu, Q^2)$ are proportional to inelastic scattering cross sections.

The small and large Q^2 limits of $W_1(0, Q^2)$ can be studied in a model-independent way. Using NRQED to compute the amplitude for double scattering of a proton in an external static magnetic field we find [17]

$$W_1(0, Q^2) = 2a_p(2 + a_p) + Q^2\{2m_p\bar{\beta}/\alpha - a_p/m_p^2 - (2/3)[(1 + a_p)^2(r_M^p)^2 - (r_E^p)^2]\} + \mathcal{O}(Q^4). \quad (11)$$

At $Q^2 \gg {\rm GeV}^2$ we may evaluate (6) using the operator product expansion (OPE). Leading terms arise from dimension-four operators and scale as Q^{-2} [17]. The intermediate Q^2 region is not constrained by existing measurements. This lack of knowledge about $W_1(0, Q^2)$ introduces model dependence in the theoretical prediction for the Lamb shift, which has so far been ignored in the literature.

Given this model dependence, how did previous studies obtain numerical predictions? The most common approach is to pretend that $W_1(0, Q^2)$ can be separated into "proton" and "nonproton" contributions. A "proton" part for $W_1(0, Q^2)$ is obtained by inserting the vertex with on-shell form factors into the Feynman diagrams for a relativistic pointlike particle. For definiteness we refer to this approach as the "Sticking In Form Factors" (SIFF) model. Explicitly,

$$W_1^{\rm SIFF}(0, Q^2) = 2F_2(2F_1 + F_2). \quad (12)$$

We emphasize that (12) is not derived from a well-defined local field theory. In fact, *no* local Lagrangian can give such Feynman rules. Note also that $W_1^{\rm SIFF}(0, Q^2)$ does not have the correct large Q^2 behavior. A "nonproton" part is obtained by multiplying the $2m_pQ^2\bar{\beta}/\alpha$ term in (11) by a function of Q^2 [21,22]. The models used in [21,22] again do not have the correct large Q^2 behavior. Unlike ${\rm Im}W_1$, we stress that the separation of $W_1(0, Q^2)$ into proton and nonproton parts is not well defined.

Bound state energies.—The use of an effective field theory allows us to systematically classify the proton structure corrections to energy levels. Using (3), proton vertex corrections, of order $(Z\alpha)^4$ and $(Z^2\alpha)(Z\alpha)^4$, are determined by c_D. Our definition (4) of the proton radius in the presence of radiative corrections implies that the $Z^2\alpha(Z\alpha)^4$ correction is unchanged from the point-particle result, so that [17]

$$\delta E^{\rm vertex}(n, \ell) = \frac{2m_r^3(Z\alpha)^4(r_E^p)^2}{3n^3}\delta_{\ell 0} + \frac{m_r^3Z^2\alpha(Z\alpha)^4}{\pi n^3} \times\left[\delta_{\ell 0}\left(\frac{4}{3}\ln\frac{m_p}{m_r\alpha^2} + \frac{10}{9}\right) - \frac{4}{3}\ln k_0(n, \ell)\right]. \quad (13)$$

Two-photon exchange corrections, of order $(Z\alpha)^5$, are determined by d_2. Considering (8), it is natural to decompose the correction as

$$\delta E^{\rm two-\gamma} = \delta E^{\rm proton} + \delta E^{\rm continuum} + \delta E^{W_1(0,Q^2)}. \quad (14)$$

It is convenient to subtract $\lim_{Q^2\to 0}W_1(0, Q^2)$ from $W_1(0, Q^2)$ in (8), and add $\lim_{Q^2\to 0}W_1(0, Q^2)$ to $W_1^{p,1}(\nu, Q^2)$. Infrared singular terms in (7) are then confined to the proton pole contribution. Having fixed this terminology, we proceed to discuss each of the three terms in $\delta E^{\rm two-\gamma}$ in turn. Our discussion so far applies to general hydrogenic bound states. To investigate numerical results we now specialize to muonic hydrogen ("μH").

Proton pole contribution.—We content ourselves with a simple dipole model for the elastic form factors,

$$G_E(q^2) \approx G_M(q^2)/G_M(0) \approx [1 - q^2/\Lambda^2]^{-2}, \quad (15)$$

where $G_E \equiv F_1 + (q^2/4m_p^2)F_2$, $G_M \equiv F_1 + F_2$ and $\Lambda^2 = 0.71\ {\rm GeV}^2$. We return to a more sophisticated analysis of this contribution, and analogous spin-dependent contributions, in forthcoming work [17]. After isolating the finite term in (7), for muonic hydrogen

$$\delta E_{\mu H}^{\rm proton}(nS) \approx (8/n^3)(0.016\ {\rm meV}). \quad (16)$$

We refrain from giving a detailed error estimation here; for the purpose of explaining the muonic hydrogen anomaly, an error smaller than 100% does not have very substantial impact.

Continuum contribution.—A recent determination of the continuum contribution is [21]

$$\delta E_{\mu H}^{\rm continuum}(nS) \approx (8/n^3)(-0.0127(5)\ {\rm meV}), \quad (17)$$

in line with previous results, $-0.014(2)$ meV [22], $-0.016(3)$ meV [23].

$W_1(0, Q^2)$ contribution.—In the SIFF model (12) one finds,

$$\delta E_{\mu H}^{W_1(0,Q^2),{\rm SIFF}}(nS) = (8/n^3)(-0.034\ {\rm meV}). \quad (18)$$

The sum of the proton pole and $W_1(0, Q^2)$ contributions in this model, $0.016\ {\rm meV} - 0.034\ {\rm meV} = -0.018\ {\rm meV}$, reproduces previous results [24]. It is not hard to construct model functions for $W_1(0, Q^2)$ that have the correct small-Q^2 and large-Q^2 behavior, but give a much larger contribution than the SIFF model.

Comparison to previous results.—In order to make the comparison to the literature clearer, we collect the results of this analysis in Table I, which compares numerical results for $\mathcal{O}(\alpha^5)$ proton structure corrections in the $2P$-$2S$ Lamb shift of muonic hydrogen. We focus on the two reference sources that were used in [2], namely [22,25]. These works model $\delta E_{\mu H}^{W_1(0,Q^2)}$ as a sum of proton and nonproton contributions, adding the respective terms to $\delta E_{\mu H}^{\text{proton}}$ and $\delta E_{\mu H}^{\text{continuum}}$. In order to simplify the comparison we present in the Table the total contribution to $\delta E_{\mu H}^{\text{two}-\gamma}$ from [22,25]. In particular for [22] we add the $(Z\alpha)^5$ nuclear size correction (0.0232 meV) and the proton polarizability correction (0.012 meV). For [25] we add the $(Z\alpha)^5$ nuclear size correction (0.0232 meV), the polarizability correction (0.015 meV), and the recoil finite size correction (0.013 meV). In [2] the nuclear size correction at order $(Z\alpha)^5$ from [22,25] employs the SIFF ansatz (12) for $W_1(0, Q^2)$; the $(r_E^p)^3$ scaling employed in [2] assumes the large m_p limit and a one-parameter model for G_E and G_M.

Let us note three differences between our results and the theoretical predictions used in [2], and collected in Table I. First, the α^5 proton vertex correction from [22,24] uses a different convention for the charge radius [26], while the result from [27], adopted in [25], uses a model-dependent SIFF prescription for the proton vertex correction; the complete result with the charge radius definition (4) is given by (13), displayed in the first line of the Table. Second, the "recoil finite size" of [25], adopted from [28], is in fact part of $\delta E_{\mu H}^{\text{two}-\gamma}$. Including it as separate contribution would lead to double counting. Third, the $\delta E_{\mu H}^{W_1(0,Q^2)}$ contribution is model dependent; the current theoretical prediction is based on the SIFF ansatz. We conclude that the dominant radiative correction to proton structure is subject to uncertainties from unreliable hadronic models.

Discussion.—We have presented the NRQED formalism for systematically analyzing proton structure effects in hydrogenic bound states. The Lamb shift in muonic hydrogen is sensitive to a new structure-dependent contact interaction (2). The strength of this interaction is not determined by measured proton form factors or inelastic structure functions. Taking all other contributions as fixed, the muonic hydrogen Lamb shift determines d_2 in (2). NRQED then predicts a universal shift for other spin-independent energy splittings in muonic hydrogen.

TABLE I. Comparison between this and previous works for $\mathcal{O}(\alpha^5)$ proton structure corrections to the $2P$-$2S$ Lamb shift in muonic hydrogen, in meV.

Contribution		Ref. [22]	Ref. [25]	This Letter	
δE^{vertex}		-0.0099	-0.0096	-0.0108	
$\delta E^{\text{two}-\gamma}$	$\delta E_{\mu H}^{\text{proton}}$	↑	↑	-0.016	
	$\delta E_{\mu H}^{W_1(0,Q^2)}$	0.035	0.051	Model Dependent	
	$\delta E_{\mu H}^{\text{continuum}}$	↓	↓	0.013	[21]
Total		0.025	0.042		

The strength of the contact interaction can be related to a so-far poorly constrained piece of the forward Compton amplitude of the proton, $W_1(0, Q^2)$. In this Letter, we have established some model-independent properties of $W_1(0, Q^2)$. First, the $\mathcal{O}(Q^2)$ Taylor expansion (11) is determined by NRQED in terms of measured quantities; second, the asymptotic behavior is determined by OPE techniques to be $\sim Q^{-2}$. The intermediate region remains poorly constrained [29]. The lack of theoretical control over $W_1(0, Q^2)$ introduces theoretical uncertainties that have not been taken into account in the literature. A common approach is to use the SIFF model (12), but this is not derived from first principles and gives the misleading impression that the dominant Q^2 dependence is constrained by on-shell form factors [21,22]. Such extrapolations represent models for $W_1(0, Q^2)$, typically without the correct large Q^2 behavior. While we do not attempt an explicit modeling of $W_1(0, Q^2)$, we believe that the uncertainty assigned to this contribution ($\lesssim 0.004$ meV [2]) is underestimated by at least an order of magnitude.

As further applications, the nonrelativistic effective theory for vector fields can similarly be employed to describe deuterium. The NRQED Lagrangian at order $1/M^4$ can be used to systematically analyze $\delta E^{\text{two}-\gamma}$ in the small-lepton mass limit relevant to electronic hydrogen, and describes spin polarizabilities of the proton [17].

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