Aspects of QED in the Framework of Exotic Atoms

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We review the status of Quantum-Electrodynamic (QED) calculations in a number of exotic hydrogen atoms. These calculations are necessary to extract from spectroscopic measurements nuclei properties like charge radius or strong interaction shifts. Different theoretical results concerning antiprotonic, pionic and muonic atoms are compared to experiments. The limitation in precision of the calculations are emphasized.

1 Introduction

The spectroscopy of exotic atoms has been used as a tool for the study of particles and fundamental properties for a long time. Exotic atoms are also interesting objects as they enable to probe aspects of atomic structure that are quantitatively different from what can be studied in electronic or "normal" atoms. For example, all exotic particles are much heavier than the electron, and thus closer to the nucleus, leading to a domination of vacuum polarization effects over self-energy contributions, in contrast to normal atoms. As an other example, pions are bosons, and thus obey the Klein-Gordon equation, while electrons and muons as spin 1/2 fermions, obey the Dirac equation. Accurate measurements of the fine structure interval in pionic atoms [1] thus offer new information compared to equivalent tests performed on hydrogen-like ions in the last 20 years [2, 3, 4].

In the present paper we review a number of examples in view of a series of recent experiments in light exotic atoms. These experiments are leading to increases of up to three orders of magnitude in the accuracy of transition energies, and thus require much more elaborate calculations.

First we will present calculations on pionic atoms, concerning a recent effort to improve the pion mass and to provide accurate strong-interaction shift and broadening in pionic hydrogen (Sec. 2). Then we will study the status of calculations of the n = 2 levels in muonic hydrogen (Sec. 3). There is an ongoing effort to measure the 2s Lamb shift in muonic hydrogen to obtain a better determination in the proton radius.

Finally we will present new results on the fine and hyperfine structure of antiprotonic hydrogen and deuterium that are required to extract information on the nucleon-antiproton interaction from measurement of Balmer $(3d \rightarrow 2p)$ transition performed at LEAR recently (Sec. 4). Section 5 contains our conclusion.

2 Pionic atoms

An accurate knowledge of the mass of the pion is useful for a number of scientific applications. For example it has been used to provide an upper limit to the muonic neutrino mass [5]. It is also necessary to extract the strong-interaction shift in pionic hydrogen [6, 7]. The most accurate way of measuring this mass is to do spectroscopy of transitions between circular states of exotic atoms, which are free of strong interaction perturbations. Extracting the pion mass from the energy of these transitions require accurate QED calculations. The use of the cyclotron trap II at the Paul Scherrer Institute (PSI) and the steady increase in pion beam intensities provides the prospect of pion to muon or pion to electron mass ratio measurement in dilute gases with accuracy at or below 1 ppm [8]. The same increase in accuracy is expected for measurements in pionic hydrogen and deuterium. In this case the extraction of reliable strong interaction shifts depend critically on the precision of the QED calculation of the np - 1s, $2 \le n \le 4$, transition energy.

The starting point of our calculation is based on the Klein-Gordon equation with a finite nucleus (uniformly charged sphere for light elements, and a two parameter Fermi model for heavy one.) We have implemented and accurate numerical solver, that has been added to the general purpose Multi-Configuration Dirac-Fock program developed by J.P. Desclaux and one of us (P.I.). This enables also to do calculation of exotic atom transition energy and lifetimes in presence of several electrons. Vacuum polarization at the Uelhing approximation (order $\alpha(Z\alpha)^4$) can be included in the radial equation, enabling to evaluate its loop-after-loop contribution to all orders (contributing to orders $\alpha^p(Z\alpha)^4$, p > 1.) The Wichmann and Kroll term (order $\alpha(Z\alpha)^6$) and the Källen and Sabry contribution, which complete the vacuum polarization contribution of order $\alpha^2 (Z\alpha)^4$ are also included. The numerical evaluation uses approximations developed in Ref. [9], exact methods from [10] and is described in more details in Ref. [11]. Recoil corrections are obtained by replacing the mass of the particle by its reduced mass, and adding first order relativistic corrections. The finite charge distribution of the pion charge is also taken into account. Good agreement is obtained in this framework with non-relativistic QED calculations (NRQED) of the pionium ($\pi^+\pi^-$ atom) [12].

As an example, we provide in Table 1 a comparison between the present work and calculation performed in Ref. [6] for pionic hydrogen. Our evaluation of the Uelhing

contribution seems to be one order of magnitude more accurate. A complete investigation of self-energy, recoil and hyperfine contributions at the 1 ppm level remains to be done. The uncalculated pion Self-energy provides the largest uncertainty. Recent attempts to do a complete QED+QCD calculation of the pionic hydrogen ground state, and of the extraction of the pion-nucleon scattering length from the experimental energy can be found, e.g., in Ref. [13] and [14].

	This work	Ref. [6]	Error
Klein-Gordon	2875.6195	2875.613	0.006
Uelhing	3.2294	3.235	
Loop-after-loop Uelhing	0.0050		
Wichmann & Kroll	0.0000		
Källèn & Sabry	0.0243		
Relativistic Recoil	0.0055		
Self-energy (estimate $[15, Eq. 30]$)	-0.0121		0.012
Uelhing (Muon pairs)	0.0002		
Recoil+Magnetic corrections		-0.047	
α^3 corrections		0.018	
Vertex		-0.007	0.003
pion recoil		-0.004	
Total	2878.8719	2878.808	0.014

Table 1: QED Contributions to pionic hydrogen $3p \rightarrow 1s$ energy. The uncertainty on the Klein-Gordon value is due to the uncertainty on the pion mass and proton charge radius

3 Muonic Hydrogen and determination of the proton radius

In the last 15 years, the accuracy of the measurement of the Rydberg constant and of the 1s - 2s and 1s - 3s transition in hydrogen has been steadily increasing. The most recent results provide a Rydberg constant accurate to 8×10^{-12} [16, 17]. For the 1s - 2stransition the accuracy has reached 1.4×10^{-14} [18]. However this impressive progress has not lead to more accurate comparison of QED calculations and experiment (Fig. 1), due to the insufficient knowledge of the proton charge distribution radius. Two different electron scattering experiments provide incompatible results. Several re-analysis of the most recent experiment have lead to several different values (see e.g., [19] and references therein.) To solve this problem, the project of measuring the $2s - 2p_{3/2}$ Lamb shift in muonic hydrogen and to deduce the proton charge distribution radius has been around for many years. While the finite charge distribution size contributes 138 ppm to the hydrogen Lamb shift, it represents 2% of the muonic hydrogen one. Recent experimental advances have lead to a large effort to realize such an experiment at PSI [20, 21]. To extract the proton charge distribution radius from the experiment with a precision of the order of 10^{-3} requires a measurement of the Lamb shift to 30 ppm. Here we review the present status of all known theoretical contributions (Table 2.)



Figure 1: Evolution of the experimental accuracy in the determination of the hydrogen Lamb shift and theoretical uncertainty due to the proton charge radius

The so-called "light by light electron-loop contribution of order $\alpha^2 (Z\alpha)^3 m$ " of table 2 is one of the largest unknown contributions to the Lamb shift in muonic hydrogen. The value of this contribution is the only one for which two incompatible orders of magnitude have been cited: below 0.001 meV [22, p. 2095], and 0.01–0.04 meV [15, § 9.3.2]. A value much greater than 0.001 meV would be larger than the "electron loop in the radiative photon" contribution (-0.0016(1) meV); this would be uncommon, since this latter contribution appears to be of lower order (see, *e.g.*, Fig. 3 in [23].)

These two results yield two different values for the $2s - 2p_{1/2}$ lamb shift. The sum of all known contributions from Table 2 with the value of [15, § 9.3.2] for the "light by light" contribution is

$$206.099(20) - 5.2256r^2 + 0.0363r^3, \tag{1}$$

where the number in parenthesis represent the uncertainty (quadratic sum), and where r, the proton mean sheprical charge radius, must be expressed in Fermi. If one uses instead Ref. [22, p. 2095], then one obtains 206.074(3) for the constant term. A new calculation of for the "light by light" contribution is thus strongly needed.

Table 2: Contributions to the $2s_{1/2} - 2p_{1/2}$ energy separation in muonic hydrogen, sorted by the size of the uncertainty. The contributions that depend on the proton radius r are numerically evaluated with r = 0.862(12) fm. EVP: electron vacuum polarization.

Diagram	Value (in meV)	Name	References
-	-3.862(108)	leading nuclear size contribution	[24, Table I], [15, § 9.6], [24, Table I]
	0.02(2)	light by light electron-loop contribution of order $\alpha^2 (Z\alpha)^3 m$	[22, p. 2095], [15, § 9.3.2]

Diagram	Value (in meV)	Name	References
<u>}</u>	0.012(2)	proton polarizability	[25], [26], [27], [24, Table I], [15, Eq. (261)]
	0.0232(15)	nuclear size correction of order $(Z\alpha)^5$	[24, Eq. (25)], [22], [27], [15, Eq. (256)], [24]
	-0.006(1)	muon self-energy with electron VP	[22, Eqs. (40) and (45)], [24, Table I], [15, Eq. (237)]
	0.0108(4)	hadronic polarization, order $\alpha(Z\alpha)^4m$	[28], [29], [30], [15, Eq. (252)], [24, Table I]
	-0.0009(3)	finite size of order α^6	[31], [32], [24, Table I], [15, Eq. (263)]
- <u></u> •	-0.0083(3)	(part of the) EVP with finite size	[33], [34], [22, Eq. (65)], [24, Table I], [15, Eq. (266)]
	-0.0126(3)	(part of the) EVP with finite size	[22, Eq. (67)], [24, Table I], [15, Eq. (268)]
	-0.0007(3)	Wichmann-Kroll, order $\alpha(Z\alpha)^4$	[22, Eq. (26)], [35], [36], [15, Eq. (231)]
	-0.0016(1)	electron loop in the radiative photon, order $\alpha^2 (Z\alpha)^4$	[37], [38], [39], [15, Eq. (242)], [40], [41], [42]
	0.0575(1)	recoil of order α^4	[43], [24, Table I], [15, Table 11]
	-0.6677(1)	$muon \ self-energy + muon \ VP$	$[24, \text{ Table I}], [15, \S 9.5]$
	-0.0440(1)	recoil corrections of order $(Z\alpha)^n \frac{m}{M}m$	$[15, \S 9.5], [24, Table I]$
	-0.0095(1)	radiative-recoil corrections of order $\alpha(Z\alpha)^n \frac{m}{M}m$	[15, § 9.5]
· ·	205.0074(1)	leading order VP	[44], [24, Table I], [15, Eq. (208)]
-0-0- 	1.5079(1)	two-loop EVP	[45], [24, Table I], [15, Eq. (213)]
-000-*	0.0053(1)	three-loop electron polarization contribution, order $\alpha^3 (Z\alpha)^2$	[46], [15, Eq. (214)], [24, Table I]
	0.1509(1)	double EVP	[24, Table I], [15, Eq. (215)], [22, Eq. (31)]
·····	0.0023(1)	polarization insertions in the two and three Coulomb lines, order $\alpha^3 (Z\alpha)^2$	[46], [15, Eq. (216)], [24, Table I]
• • • • • • • • • • • • • • • • • • •	0.0005(1)	radiative correction to the nuclear finite size	[15, Eq. (264)], [47]
	-0.0099(1)	proton self-energy	[24, Table I]

Table 2: Contributions to the $2s_{1/2} - 2p_{1/2}$ transition energy in muonic hydrogen (continued)

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Diagram	Value (in meV)	Name	References
	0.0594(1)	relativistic correction to the	[22], [24, Table I], [15,
		EVP	Eq. (223)]
	0.00007(1)	mixed electron and muon	
		loops, order	[48], [15, Eq. (248)]
×		$\alpha^2 (Z\alpha)^2 (m_e/m)^2 m$	
<u> </u>	-0.000015(1)	hadronic polarization in the	
		radiative photon, order	[30], [15, Eq. (254)]
		$\alpha^2 (Z\alpha)^4 m$	
· · · ·	0.000047(1)	hadronic polarization, order	[30] $[15$ Eq. $(253)]$
		$lpha(Zlpha)^5m$	[50], [10, 124. (200)]

Table 2: Contributions to the $2s_{1/2} - 2p_{1/2}$ transition energy in muonic hydrogen (continued)

4 Fine and hyperfine structure of antiprotonic Hydrogen and Deuterium

The availability of very low energy antiprotons LEAR has lead to many experiments involving antiprotonic atoms. Just before the shudtdown of LEAR, high resolution X-ray spectroscopy of $n = 3 \rightarrow n = 2$ transitions in antiprotonic hydrogen H⁺ \bar{p} and deuterium D⁺ \bar{p} has been performed [49]. The aim of such experiments is to provide high accuracy strong-interaction shifts and broadenings. These shifts can provide accurate *s* and *p*-wave scattering cross-section for nucleon-antinucleon interaction at very low energy, and are thus of fundamental importance. The antiproton is a spin 1/2 composite particle, the gyro-magnetic ratio of which $g_{\bar{p}} = -5.585694772(126)$ [50] is very different from the value predicted for an elementary particle like the electron (| $g \approx 2$.)

In the present work we report on an accurate calculation, which include all the recoil and Vacuum polarization corrections described in Sec. 2. To that we add Hyperfine corrections to account for the interaction between the magnetic moment of the nucleus and the orbital and intrinsic moment of the antiproton. We add the corrections due to the anomalous magnetic moment of the antiproton as well. This is done by introducing the operator (valid for distances larger than the Compton wavelength of the electron \hbar/mc)

$$\Delta H = a \frac{\hbar q}{2m_p} \beta \left(i \frac{\boldsymbol{\alpha} \boldsymbol{E}}{c} - \boldsymbol{\Sigma} \boldsymbol{B} \right).$$
⁽²⁾

where a is defined by a = (g - (-2))/2 for an antiparticle of negative charge q, m_p is the antiproton mass, E and B are the electric and magnetic fields generated by the nucleus, α are Dirac matrices and

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\sigma} \end{pmatrix}. \tag{3}$$

For the antiproton we thus have $a_{\bar{p}} = -1.792847386$ in place of $-\alpha/(2\pi)$ for a positron.

The calculation shows that fine structure, hyperfine structure and g - 2 contributions are of the same order of magnitude. In order to account to higher-order effects, we thus calculate for each group of level $2p_j$ or $3d_j$ the complete Hamiltonian matrix corresponding to Hyperfine and g-2 corrections, including all non-diagonal matrix elements. The matrix is then diagonalized to obtain the final energy. The results for antiprotonic hydrogen and deuterium are presented in Figs. 2 and 3. The agreement between these new calculation and experiment is much better than with previous work [51], which do not enable to reproduce the observed line shape.



Figure 2: Structure of the contributions to the 2p levels of antiprotonic Hydrogen. Borie: [52].



Figure 3: Structure of the contributions to the 2p levels of antiprotonic Deuterium . Pilkuhn: [53].

5 Conclusion

In this review we have presented a number of new BSQED results together with existing calculations of transition energies in exotic hydrogen atoms. The best known case is indeed muonic hydrogen, although more work is needed for at least one contribution. In view of advances in the spectroscopy of pionic hydrogen, much effort should be done to improve the status of the calculation. Antiprotonic hydrogen and deuterium exhibit a very intresting fine structure that has been investigated in detail for the present work, but wich requires new developments to be understood completely at a level compatible with experiment.

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