Higher-order recoil corrections in Helium and Helium-like ions

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19th May 2017

Motivation

- Hydrogenic systems such as H, He^{+} or μH are being considered for low-energy tests of the Standard model and for determination of fundamental constants
- Comparison of accurate experimental values for transition frequencies with theoretical predictions gives us information about the extent to which energy levels can by predicted by the Standard model
- Any discrepancy would be signal of new physics or incorrect values of physical constants

- One can reverse the problem and use the comparison of experimental values with theoretical predictions to extract values of fundamental constants
- Example of this is using the measurement of anomalous magnetic moment of bound electron in H-like carbon ions with high precision theoretical predictions for determination of electron mass
- This method improves the accuracy for determination of electron mass by two orders of magnitude

- Another example is comparison of the Lamb shift in muonic hydrogen with electronic one
- This provides us with significantly different values of proton charge radius

$$\sqrt{\langle r_p^2 \rangle}_{eH} = 0.8770(45)\, fm$$
$$\sqrt{\langle r_p^2 \rangle}_{\mu H} = 0.8409(4)\, fm$$

- Existence of interactions that are not accounted for?
- Lack of universality in lepton-hadron interaction?
- Incorrect values of physical constants?

- Recent results indicates that value of Rydberg constant is incorrect and previous hydrogen measurements were not as accurate as claimed and same holds for determination of r_p from proton scattering
- This still requires further confirmation
- Another experiment aimed in resolving the proton radius puzzle is the direct comparison of the $e - p$ to $\mu - p$ scattering cross section

- Present electronic and muonic hydrogen theory allows accurate determination of the proton charge radius from measured transition frequencies, and the comparison between electronic and muonic results stands as a low-energy test of the Standard Model
- Purpose of our calculations is to bring the high accuracy achieved for hydrogenic levels to few-electron atomic and molecular systems and in particular for helium and helium-like ions

- Contribution of the nuclear finite size effect to energy levels is

$$\delta_{fs}E = \frac{2\pi Z\alpha}{3}\phi^2(0)\langle r_{ch}^2\rangle = C\langle r_{ch}^2\rangle$$

- Determination of the nuclear charge radius comes from

$$\langle r_{ch}^2\rangle = \frac{E_{exp} - E_{theo}}{C}$$

- For $2^3S - 2^3P$ transition in ^4He $\delta_{fs}E \simeq 3.5$ MHz. To obtain r_{ch} with accuracy of few parts in 10^{-3} one has to calculate the transition energies on 10 kHz level.

Case of hydrogen

- Dirac equation (with infinite nuclear mass)
- One-loop self-energy and vacuum polarization

$$E = \frac{\alpha}{\pi}(Z\alpha)^4\Big[A_{40} + (Z\alpha)\,A_{50} + (Z\alpha)^2\left(A_{62}\ \ln^2(Z\alpha)^{-2} + A_{61}\ \ln(Z\alpha)^{-2} + A_{60} + \cdots\right.$$

- Two-loop correction

$$E = \left(\frac{\alpha}{\pi}\right)^2(Z\alpha)^4\Big[B_{40} + (Z\alpha)\,B_{50} + (Z\alpha)^2\left(B_{63}\ \ln^3(Z\alpha)^{-2} + B_{62}\ \ln^2(Z\alpha)^{-2} + +B_{61}\ \ln(Z\alpha)^{-2} + B_{60}\right.$$

- Recoil corrections

Case of helium

- Calculation of relativistic corrections to energy levels of atomic systems is usually acomplished by using many-electron Dirac-Coulomb Hamiltonian with possible inclusion of Breit interaction between electrons
- Such a Hamiltonian can not be rigorously derived from QED and thus gives incomplete treatment of relativistic and QED effects
- Electron self-energy and vacuum polarization can be included in the DC Hamiltonian, although only in approximate way

NRQED

Alternative approach called Non-relativistic Quantum electrodynamics relies on expansion of energy levels in powers of the fine structure constant

$$E(\alpha) = E^{(2)} + E^{(4)} + E^{(5)} + E^{(6)} + E^{(7)} + \cdots , \; E^{(n)} \sim m\,\alpha^n$$

All expansion terms are expressed in terms of expectation values of some effective Hamiltonian with nonrelativistic wave function

Every term is then expanded in powers of the electron-to-nucleus mass ratio m/M

$$E^{(n)} = E^{(n)}_{\infty} + \frac{m}{M}\,\delta_M E^{(n)} + O\Big(\frac{m}{M}\Big)^2$$

$E^{(2)}$ is a nonrelativistic energy corresponding to the Hamiltonian

$$H^{(2)} = \sum_a \left(\frac{\vec{p}_a^{\,2}}{2m} - \frac{Z\alpha}{r_{aI}}\right) + \sum_{a>b}\sum_b \frac{\alpha}{r_{ab}} + \frac{\vec{P}_I^{\,2}}{2M}$$

$E^{(4)}$ is leading relativistic correction,

$$E^{(4)} = \langle H^{(4)} \rangle$$

$$\begin{aligned} H^{(4)} &= \sum_a \left[-\frac{\vec{p}_a^{\,4}}{8\,m^3} + \frac{\pi\,Z\,\alpha}{2\,m^2}\,\delta^3(r_{aI}) + \frac{Z\,\alpha}{4\,m^2}\,\vec{\sigma}_a \cdot \frac{\vec{r}_{aI}}{r_{aI}^3} \times \vec{p}_a \right] \\ &+ \sum_{a<b} \Bigg\{ -\frac{\pi\,\alpha}{m^2}\,\delta^3(r_{ab}) - \frac{\alpha}{2\,m^2}\,p_a^i \left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3} \right) p_b^j \\ &- \frac{2\pi\,\alpha}{3\,m^2}\,\vec{\sigma}_a \cdot \vec{\sigma}_b\,\delta^3(r_{ab}) + \frac{\alpha}{4\,m^2}\,\frac{\sigma_a^i\,\sigma_b^j}{r_{ab}^3} \left(\delta^{ij} - 3\,\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^2} \right) \\ &+ \frac{\alpha}{4\,m^2\,r_{ab}^3} \big[2\,(\vec{\sigma}_a \cdot \vec{r}_{ab} \times \vec{p}_b - \vec{\sigma}_b \cdot \vec{r}_{ab} \times \vec{p}_a) \\ &+ (\vec{\sigma}_b \cdot \vec{r}_{ab} \times \vec{p}_b - \vec{\sigma}_a \cdot \vec{r}_{ab} \times \vec{p}_a) \big] \Bigg\} \end{aligned}$$

$E^{(5)}$ stands for the leading QED correction,

$$\begin{aligned} E^{(5)} &= \left[\frac{164}{15} + \frac{14}{3}\right] \ln\alpha\Big] \frac{\alpha^2}{m^2}\langle\delta^3(r_{12})\rangle \\ &+ \left[\frac{19}{30} + \ln(Z\alpha)^{-2}\right] \frac{4\alpha^2 Z}{3\,m^2}\langle\delta^3(r_1) + \delta^3(r_2)\rangle \\ &- \frac{14}{3}\, m\alpha^5 \left\langle \frac{1}{4\,\pi}\, P\left(\frac{1}{(m\alpha\, r_{12})^3}\right)\right\rangle \\ &- \frac{2\,\alpha}{3\,\pi\, m^2}\left\langle \sum_a \vec{p}_a (H^{(2)} - E^{(2)})\, \ln\left[\frac{2(H^{(2)} - E^{(2)})}{(Z\alpha)^2\, m}\right] \sum_b \vec{p}_b \right\rangle \end{aligned}$$

Higher-order term $E^{(6)}$ consists of two parts,

$$E^{(6)} = \langle H^{(6)} \rangle + \left\langle H^{(4)} \frac{1}{(E^{(2)} - H^{(2)})'} H^{(4)} \right\rangle$$

Here

$$H^{(6)} = \sum_{i=1..11} H_i$$

Both parts contain singular operators like r_{12}^{-3}, r_{12}^{-4} etc

- It is necessary to perform regularization in order to isolate singular parts of all terms. These singularities eventually cancel each other
- Particular regularization scheme we choose is dimensional regularization

$$d = 3 \to d = 3 - 2\epsilon$$

- All the singularities $\propto \frac{1}{\epsilon}$ then cancel each other

- After simplification the terms are expressed in terms of operators $Q_1, Q_2, \cdots, Q_{55}$ which are suitable for numeric calculation

$$
\begin{aligned}
Q_1 &= 4\pi\delta^3(r_1) \\
Q_2 &= 4\pi\delta^3(r_{12}) \\
Q_3 &= 4\pi\delta^3(r_1)/r_2 \\
Q_4 &= 4\pi\delta^3(r_1)\, p_2^2 \\
Q_5 &= 4\pi\delta^3(r_{12})/r_1 \\
Q_6 &= 4\pi\, \vec{p}\,\delta^3(r_{12})\,\vec{p},\ \vec{p} = (\vec{p}_1 - \vec{p}_2)/2 \\
Q_7 &= 1/r_{12} \\
Q_8 &= 1/r_{12}^2 \\
&\cdots
\end{aligned}
$$

- For the Helium wave function we use expansion in the bases set of exponential functions of the Korobov type,

$$\phi(^3S) = \sum_{i=1}^{\mathcal{N}} v_i \left[e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r} - (r_1 \leftrightarrow r_2)\right]$$

$$\phi(^3P) = \sum_{i=1}^{\mathcal{N}} v_i \left[\vec{r}_1\, e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r} - (r_1 \leftrightarrow r_2)\right]$$

$$\phi(^1S) = \sum_{i=1}^{\mathcal{N}} v_i \left[e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r} + (r_1 \leftrightarrow r_2)\right]$$

$$\phi(^1P) = \sum_{i=1}^{\mathcal{N}} v_i \left[\vec{r}_1\, e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r} + (r_1 \leftrightarrow r_2)\right]$$

- The calculation of matrix elements of the nonrelativistic Hamiltonian is based on the single master integral,

$$\frac{1}{16\pi^2}\int d^3r_1\int d^3r_2\,\frac{e^{-\alpha r_1-\beta r_2-\gamma r}}{r_1\,r_2\,r}=\frac{1}{(\alpha+\beta)(\beta+\gamma)(\gamma+\alpha)}$$

- The integrals with any additional powers of r_i in the numerator can be obtained by differentiation with respect to the corresponding parameter α, β or γ

Results

Theoretical contributions to the centroid ionization energy of 1^1S state in ^{4}He, in MHz.

	$(m/M)^0$	$(m/M)^1$	$(m/M)^2$	$(m/M)^3$	Sum
α^2	−5 946 220 752.325	958 672.945	−209.270	0.049	−5 945 262 288.601
α^4	16 904.024	−103.724	0.028		16 800.327
α^5	40 506.158	−10.345			40 495.813
α^6	861.360	−0.348			861.012
α^7	−71. (36.)				−71. (36.)
NS	29.7 (1)				29.7 (1)
Total					−5 945 204 173. (36.)

K. Pachucki, V. Patkóš, V. A. Yerokhin: Testing fundamental interactions on the helium atom, sent to Phys. Rev. A

Comparison of the theoretical predictions for various transitions in ^{4}He with the experimental results, in MHz.

	Theory	Experiment
1^1S	5 945 204 173 (36)	5 945 204 212 (6)
1^1S–2^1S	4 984 872 135 (36)	4 984 872 315 (48)
2^3S–3^3D_1	786 823 848.4 (1.3)	786 823 850.002 (56)
2^1S–2^1P_1	145 622 891.5(2.3)	145 622 892.886 (183)
2^1P_1–3^1D_2	448 791 397.4(0.4)	448 791 399.113 (268)
2^3P_0–3^3D_1	510 059 754.0 (0.7)	510 059 755.352 (28)
2^3P–2^3S	276 736 495.4 (2.0)	276 736 495.649 (2)
2^3S–2^1P_1	338 133 594.9 (1.4)	338 133 594.4 (5)
2^1S–2^3S	192 510 703.4 (0.8)	192 510 702.145 6 (18)

$^3\mathrm{He} - {}^4\mathrm{He}$ isotope shift of the 2^3S–2^3P centroid transition energy in kHz

	$(m/M)^1$	$(m/M)^2$	$(m/M)^3$	Sum
α^2	33 673 018.7	−3 640.6	0.4	33 669 378.5
α^4	−2 214.9	−2.4	—	−2 217.3
α^5	−60.7	—	—	−60.7
α^6	−9.4	—	—	−9.4
α^7	0.0 (0.9)	—	—	0.0 (0.9)
NPOL	−1.1	—	—	−1.1
EMIX	—	54.6	—	54.6
Total				33 667 149.3(0.9)

$$\delta r_{ch}^2\,(\mathrm{Florence\,2012},\ 2^3P - 2^3S) = 1.069\,(3)\,\mathrm{fm}^2$$
$$\delta r_{ch}^2\,(\mathrm{Shiner\,1995},\ 2^3P - 2^3S) = 1.061\,(3)\,\mathrm{fm}^2$$
$$\delta r_{ch}^2\,(\mathrm{Amsterdam\,2011},\ 2^1S - 2^3S) = 1.027\,(11)\,\mathrm{fm}^2$$

V. Patkóš, V. A. Yerokhin and K. Pachucki, Phys. Rev. A 95, 012508 (2017)
V. Patkóš, V. A. Yerokhin and K. Pachucki, Phys. Rev. A 94, 052508 (2016)

Conclusions

- By calculating the higher-order terms $E^{(6)}$ and $E^{(7)}$ we will achieve the same accuracy of theoretical calculations for helium as in the hydrogenic case
- Such an accuracy will enable us to get absolute nuclear charge radius and in general to carry out low-energy tests of Standard model and its extensions
- The next step is to calculate contribution of the leading term in $E^{(7)}$ contribution
- Further application is to calculate leading $E^{(6)}$ contribution for Lithium atom

Collaborators

- Krzysztof Pachucki, University of Warsaw
- Vladimir A. Yerokhin, St. Petersburg Technical university
- Jaroslav Zamastil, Charles University in Prague