Higher-order QED corrections in two-body systems

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QED of two-body systems

- The highest precision for theoretical determination of atomic spectra can be achieved for two-body systems
- Combined with precise experimental data we may obtain very accurate values of fundamental constants or constraints on physics beyond the Standard Model
- Two-body systems like hydrogen, heavy ions, muonium, positronium, He^+ and even more challenging like antiprotonic hydrogen and helium can be available experimentally

- One may replace proton or electron in hydrogenlike atoms by other particles such as alpha, pion, positron, muon or antiproton
- For highly excited rotational states the strong interaction effects are negligible
- The only limiting factor on theory would be uncertainty of Rydberg constant, mass ratio, magnetic moment anomaly, polarizability

- For obtaining theoretical prediction for atomic spectra we use Nonrelativistic QED (NRQED), perturbative method in which the energy is expressed as power series

$$E = E^{(2)} + E^{(4)} + E^{(5)} + E^{(6)} + E^{(7)} + O(\alpha^8)$$

with $E^{(j)}$ being of the order α^j

- Each term can be expressed as an expectation value of some effective operator with nonrelativistic wave function

$$E^{(2)} \equiv E_0 = -\frac{(Z\alpha)^2\,\mu}{2n^2}$$

- Leading relativistic correction $E^{(4)}$ is expectation value of Breit Hamiltonian

$$
\begin{aligned}
E^{(4)} =& \mu^3 (Z\alpha)^4 \Bigg\{ \frac{1}{8\,n^4} \left(\frac{3}{\mu^2} - \frac{1}{m_1\, m_2} \right) - \frac{1}{\mu^2 (2l+1)\, n^3} \\
& + \frac{2}{l(l+1)(2l+1) n^3} \Bigg[\vec{L}\cdot\vec{s}_1 \left(\frac{1+2\kappa_1}{2 m_1^2} + \frac{1+\kappa_1}{m_1 m_2} \right) \\
& + \vec{L}\cdot\vec{s}_2 \left(\frac{1+2\kappa_2}{2 m_2^2} + \frac{1+\kappa_2}{m_1 m_2} \right) - \frac{6(1+\kappa_1)(1+\kappa_2)}{m_1 m_2\,(2\,l-1)(2\,l+3)} \\
& \times s_1^i s_2^j (L^i L^j)^{(2)} \Bigg] \Bigg\}
\end{aligned}
$$

for $l > 0$, where $g = 2(1+\kappa)$

- Contribution $E^{(5)}$ contains leading QED corrections, is partially accounted for in the g-factor and is known in the literature

- Next-order correction is a higher-order QED contribution $E^{(6)}$ which is a sum of two parts

$$E^{(6)} = \langle H^{(6)} \rangle + \langle H^{(4)} \frac{1}{(E_0 - H_0)'} H^{(4)} \rangle$$

- First-order operator $H^{(6)} = \sum_{i=0}^{9} \delta H_i$ is derived in the NRQED framework

- For S states and two spin-1/2 particles of arbitrary masses the result was obtained recently by G. Adkins et al., Phys. Rev. Lett. 130, 023004 (2023)

- For $l > 0$ the result can be written in a form

$$E^{(6)} = \frac{\mu\,(Z\alpha)^6}{l(l-1)(2l-1)(2l+1)(2l+3)}\Big[A + B\,\vec{L}\cdot\vec{s}_1 + C\,\vec{L}\cdot\vec{s}_2 + D\,\vec{s}_1\cdot\vec{s}_2 + F\,s_1^i s_2^j\,(L^i L^j)^{(2)}\Big]$$

- For $l > 1$ we performed the calculation in Phys. Rev. A **106**, 042804 (2022)

- Coefficients $A - F$ are in general quite complicated expressions, the result is valid for either spin 0 or 1/2, pointlike or hadronic particles and arbitrary masses
- In special cases (hydrogen, positronium) the results are in agreement with known results in the literature (Dirac equation and leading recoil correction, Klein-Gordon equation)
- Derived formulas can be applied to various exotic atoms

- Recently we extended the calculation also to P states, Phys. Rev. A **109**, 022819 (2024)

- For P states there is nonvanishing local interaction proportional to $\vec{p}\,\delta^3(r)\,\vec{p}$ and the results depend also on charge and magnetic radii of both particles

- For instance, in the case of hydrogen atom in nonrecoil limit the result is

$$E^{(6,0)} = m_2\,(Z\alpha)^6\biggl\{\biggl(-\frac{5}{16\,n^6}+\frac{1}{2\,n^5}-\frac{3}{16\,n^4}-\frac{5}{96\,n^3}\biggr) + \vec{L}\cdot\vec{s}_2\biggl(-\frac{1}{4\,n^5}+\frac{3}{16\,n^4}+\frac{7}{96\,n^3}\biggr) + \frac{1}{9}\biggl(\frac{1}{n^3}-\frac{1}{n^5}\biggr)\biggl[\biggl(\frac{1}{2}-\vec{L}\cdot\vec{s}_2\biggr)m_2^2\,r_{E1}^2+\frac{1}{5}\,m_2^4\,r_{EE1}^4\biggr]\biggr\}$$

- We found out that our results for P states and the general result with l set to $l = 1$ differ in the point particle limit

- This affects the results for positronium atom, leading to discrepancy in theoretical results

- This difference is

$$\delta E_{\rm pos} = E^{(6)} - E_G^{(6)}\Big|_{l=1, m_1=m_2}$$
$$= \frac{m\,(Z\alpha)^6}{32}\left(\frac{1}{n^3} - \frac{1}{n^5}\right)\left(\frac{1}{24} - \frac{\vec{L}\cdot(\vec{s}_1+\vec{s}_2)}{12} + \frac{\vec{s}_1\cdot\vec{s}_2}{18} + \frac{(L^i L^j)^{(2)}\, s_1^i s_2^j}{3}\right)$$

- For particular positronium states this ammounts to

$$\delta E_{\mathrm{pos}}(s=0, j=1) = 0$$
$$\delta E_{\mathrm{pos}}(s=1, j=0) = \frac{m\,(Z\alpha)^6}{64}\left(\frac{1}{n^3} - \frac{1}{n^5}\right)$$
$$\delta E_{\mathrm{pos}}(s=1, j=1) = 0$$
$$\delta E_{\mathrm{pos}}(s=1, j=2) = 0$$

- The corresponding numerical change is too small to affect comparison with experiment

- Application of general formulas: $2P$ fine structure in μHe ion

- Leading contribution is

$$E_{\rm fs}^{(4)} = \frac{\mu^3 (Z\alpha)^4}{32} \left(\frac{g_\mu - 1}{m_\mu^2} + \frac{g_\mu}{m_{\rm N}\, m_\mu} \right)$$

- Correction of order α^6 is obtained for both spinless and spin-1/2 nucleus

- For this correction we may set $g_\mu = 2$ and omit QED corrections to r_E and r_M of the muon

- For spinless nucleus the fine structure of $2P$ state is

$$E_{\rm fs}^{(6)} = \mu\,\frac{(Z\,\alpha)^6}{64}\,\biggl[\frac{5}{4} + \frac{1}{4}\,\frac{\mu}{m_N} - \frac{19}{18}\,\Bigl(\frac{\mu}{m_N}\Bigr)^2 - \frac{3}{4}\,\Bigl(\frac{\mu}{m_N}\Bigr)^3 + \frac{11}{36}\,\Bigl(\frac{\mu}{m_N}\Bigr)^4 - \mu^2\,r_E^2\,\Bigl(1 - \frac{\mu^2}{m_N^2}\Bigr)\biggr]$$

- For spin-1/2 nucleus it is

$$E_{\rm fs}^{(6)} = \mu\,\frac{(Z\,\alpha)^6}{64}\,\biggl[\frac{5}{4} + \frac{1}{4}\,\frac{\mu}{m_N} + \Bigl(-\frac{19}{18} + \frac{2729}{3600}\,g_N^2\Bigr)\Bigl(\frac{\mu}{m_N}\Bigr)^2 + \Bigl(-\frac{3}{4} + \frac{5}{72}\,g_N - \frac{188}{225}\,g_N^2\Bigr)\Bigl(\frac{\mu}{m_N}\Bigr)^3 + \Bigl(\frac{11}{36} - \frac{5}{72}\,g_N + \frac{31}{400}\,g_N^2\Bigr)\Bigl(\frac{\mu}{m_N}\Bigr)^4 - \mu^2\Bigl(r_E^2 + \frac{3}{4\,m_N^2}\Bigr)\Bigl(1 - \frac{\mu^2}{m_N^2}\Bigr)\biggr]$$

contribution	$\mu^3\text{He}^+$	$\mu^4\text{He}^+$
$E_{\rm fs}^{(4)}$	144.510 95	145.898 24
$E_{\rm fs,vp}^{(4)}$	0.269 81	0.275 65
$E_{\rm fs}^{(6)}$	0.004 05	0.007 64
$E_{\rm fs}$	144.785(3)	146.182(3)
Refs [a,b]	144.785(5)	146.181(5)
Refs [c,d]	144.763(114)	146.047(96)

[a] S. G. Karshenboim, E. Yu. Korzinin, V. A. Shelyuto, and V. G. Ivanov, Phys. Rev. A **96**, 022505 (2017);
[b] E. Yu. Korzinin, V. A. Shelyuto, V. G. Ivanov, and S. G. Karshenboim, Phys. Rev. A **97**, 012514 (2018);
[c] K. Schuhmann et al., arXiv:2305.11679;
[d] R. Pohl et al., Science 353, 669 (2016)

- Our results are in agreement with previous calculations and with experimental results. The observed agreement supports the determination of the nuclear charge radii reported in these works

- Additionaly, we have checked our results for nuclear recoil correction for muonic atoms by the all-order calculation (talk of Vladimir Yerokhin)

$E^{(7)}$ radiative corrections

- To improve theoretical accuracy further we may include also contribution of order α^7

- It is given by the expression

$$E^{(7)} = E_L + \langle H^{(7)} \rangle + 2 \left\langle H^{(4)} \frac{1}{(E_0 - H_0)'} H^{(5)} \right\rangle$$

- We calculated one-loop radiative corrections for $l > 0$ states of two-body systems with spin-1/2 particles, with pointlike or hadronic nucleus, and arbitrary masses

- The contribution $E_{\rm rad}^{(7)}$ can be expressed as

$$E_{\rm rad}^{(7)} = \frac{\mu\,\alpha(Z\alpha)^6}{\pi\, l(l-1)(2l-1)(2l+1)(2l+3)} \times \left[A + B\,\vec{L}\cdot\vec{s}_1 + C\,\vec{L}\cdot\vec{s}_2 + D\,\vec{s}_1\cdot\vec{s}_2 + F\,s_1^i s_2^j\,(L^i L^j)^{(2)}\right]$$

- General formulas again complicated but specific cases are more compact
- Preliminary unpublished results

- For hydrogen P states in nonrecoil limit it is

$$
\begin{aligned}
E^{(7,0)}_{\rm hydr}(nP) = \frac{m_1\,\alpha(Z\alpha)^6}{\pi}\biggl(&\frac{1319}{3600\,n^3} - \frac{1}{24\,n^4} - \frac{1687}{5400\,n^5}\\
&+ \langle\vec{L}\cdot\vec{s}_1\rangle\left(\frac{1}{80\,n^3} + \frac{5}{24\,n^4} - \frac{135}{135\,n^5}\right) + \left(\frac{23}{45\,n^3} - \frac{19}{45\,n^5}\right.\\
&- \frac{2}{9}\left(\langle\vec{L}\cdot\vec{s}_1\rangle - \frac{2}{3}\,m_1^2\,r_{E2}^2\right)\left.\frac{(n^2-1)}{n^5}\right)\ln\left[\tfrac{1}{2}(Z\alpha)^{-2}\right]\\
&+ \left(\frac{10}{81} - \frac{1}{9}\,\langle\vec{L}\cdot\vec{s}_1\rangle\right)\frac{(n^2-1)}{n^5}\,m_1^2\,r_{E2}^2\\
&+ \frac{1}{n^3}\left(\beta_{\rm NS}(0) + \langle\vec{L}\cdot\vec{s}_1\rangle\,\beta_{\rm S1}(0)\right)\biggr)
\end{aligned}
$$

- In agreement with work U. D. Jentschura, A. Czarnecki, and K. Pachucki, Phys. Rev. A **72**, 062102 (2005) in pointlike limit

- For positronium P states the results are

$$E^{(7)}_{\rm pos}(n^S P_J) = \frac{\alpha(Z\alpha)^6\, m}{\pi}\left(\delta E^{(7)}(n^S P_J) + \frac{(3n^2-2)}{90\, n^5}\right.$$
$$\left.\times\left(H_{n+1} - \ln\frac{n}{Z\alpha}\right)\right)$$

where $H_n = \sum_{i=1}^{n} i^{-1}$ gives the n-th harmonic number

-

$$\delta E^{(7)}(n^1 P_1) = \frac{\beta^{\rm pos}(^1P_1)}{n^3} + \frac{73}{1440\, n^3} - \frac{1}{20\, n^4} - \frac{47}{3600\, n^5}$$
$$+ \left(\frac{3}{40\, n^3} - \frac{19}{360\, n^5}\right)\ln\left[\tfrac{1}{2}(Z\alpha)^{-2}\right]$$

$$\delta E^{(7)}(n^3P_0) = \frac{\beta^{\rm pos}(^3P_0)}{n^3} - \frac{101}{960\,n^3} - \frac{3}{10n^4} + \frac{307}{2400\,n^5} + \left(\frac{29}{120\,n^3} - \frac{79}{360\,n^5}\right)\ln\left[\tfrac{1}{2}(Z\alpha)^{-2}\right]$$

$$\delta E^{(7)}(n^3P_1) = \frac{\beta^{\rm pos}(^3P_1)}{n^3} + \frac{181}{1728n^3} - \frac{73}{960n^4} - \frac{877}{21600n^5} + \left(\frac{47}{360\,n^3} - \frac{13}{120\,n^5}\right)\ln\left[\tfrac{1}{2}(Z\alpha)^{-2}\right]$$

$$\delta E^{(7)}(n^3P_2) = \frac{\beta^{\rm pos}(^3P_2)}{n^3} + \frac{491}{8000\,n^3} - \frac{41}{1600\,n^4} - \frac{67}{900\,n^5} + \left(\frac{3}{40\,n^3} - \frac{19}{360\,n^5}\right)\ln\left[\tfrac{1}{2}(Z\alpha)^{-2}\right]$$

- If we set both particles to be electrons then we may compare results for effective operators with two-body electron-electron part of our helium calculation for triplet states, Phys. Rev. A **103**, 012803 (2021)
- We found a mistake in our helium calculations, however it ammounts only to few kHz
- Still no explanation for discrepancy in ionization energies of helium triplet states

Summary

- The most precise theoretical predictions can be obtained from two-body systems
- We obtained formulas valid for arbitrary pointlike or hadronic particles with spin either zero or $1/2$, and $l > 0$
- We extended the calculation also to α^7 radiative correction
- In the future we also have to account for the photon-exchange contribution of the order α^7
- For rotational states with $n \approx l + 1$ the effective coupling constant is $Z\alpha/n$ so we can apply these results to heavy ions

Thank you for your attention!