Testing fundamental interactions with few electron atoms and molecules

Krzysztof Pachucki

University of Warsaw

Physics of Fundamental Symmetries and Interactions
PSI2016, October 17

Motivation and challenges

Motivations

- *the interface between the strong and electromagnetic interactions, can be probed very accurately in atomic physics*
- how come r_p from (electronic) H differs by 4% from that of μH ?
- violation of lepton universality of SM ?
- incorrect Ry constant ?
  - muonium 1S-2S + HFS, muon life time 2.2 μs
  - He^+(1S-2S), T. Udem (Garching), K. Eikema (Amsterdam)
  - highly excited states of heavy hydrogen-like ions (NIST)

Few electron atomic and molecular systems

The general purpose of our project is to bring the high accuracy achieved for hydrogenic levels to few-electron atomic and molecular systems

- for the determination of the nuclear charge radii from experimental transition frequencies
- to search for any discrepancies with spectroscopic measurements and uncover unknown forces at the atomic scale
- to carry out low-energy tests and of various extensions of the Standard Model of fundamental interactions
- determination of fundamental constants Ry, α

$$f(1S-2S,H) = 2\,466\,061\,413\,187\,035(10)\mathrm{Hz} \qquad (\sim 10^{-16})$$

lack of second sharp transition in H

- H_2 dissociation energy F. Merkt (ETH) + W. Ubachs (Amsterdam)

The nuclear finite size effect

- $\delta_{\rm fs} E = \frac{2\,\pi\,Z\,\alpha}{3}\,\phi^2(0)\,\langle r_{ch}^2\rangle = C\,\langle r_{ch}^2\rangle$
- this formula is universal, valid for an arbitrary atomic system
- higher order $O(Z\,\alpha\,r_{\rm ch}/\lambda\!\!\!^{-})$, small for electronic atoms
- determination of mean square nuclear charge radius from:

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

α charge radius from He $2^3S - 2^3P$

- $E(2^3S - 2^3P, {}^4\mathrm{He})_{\mathrm{centroid}} = 276\,736\,495\,649.5(2.1)$ kHz, Florence, 2004
- finite size effect: $E_{\mathrm{fs}} = 3\,427$ kHz
- since E_{fs} is proportional to r^2

$$\frac{\Delta r}{r} = \frac{1}{2}\frac{\delta E_{\mathrm{fs}}}{E_{\mathrm{fs}}} \approx \frac{1}{2}\frac{10}{3\,427} = 1.5 \cdot 10^{-3}$$

- electron scattering gives $r_{\mathrm{He}} = 1.681(4)$ fm, what corresponds to about $2.5 \cdot 10^{-3}$ relative accuracy
- $\sim$ 10 kHz accuracy requires calculation of $m\alpha^7$ correction

r_P from dissociation energy of H_2

- $D_0(H_2) = 36118.06962(37)\ \mathrm{cm}^{-1}$, J. Liu at al, 2009
- at the $6 \cdot 10^{-7}\ \mathrm{cm}^{-1}$ accuracy for H_2 levels
- the proton charge radius which contributes $3.1\,10^{-5}\ \mathrm{cm}^{-1}$ to the dissociation energy can be determined to 1.0% accuracy (discrepancy is at 4%)
- requires calculation of $m\,\alpha^7$ and the so called nonadiabatic corrections.

Hydrogen theory

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

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

or directly numerically, known very accurately

- two-loop correction

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

B_{60} is not very accurate, main source of the uncertainty, a few kHz for 1S

- pure (Shabaev formula) and radiative recoil

NRQED approach to few electron systems

Atomic energy levels are expanded in powers of the fine structure constant α

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

NRQED approach to few electron systems

Atomic energy levels are expanded in powers of the fine structure constant α

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

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

$$H^{(2)} = \sum_a \frac{\vec{p}_a^{\,2}}{2\,m} - \frac{Z\,\alpha}{r_a} + \sum_{a>b} \frac{\alpha}{r_{ab}}$$

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

NRQED approach to few electron systems

Atomic energy levels are expanded in powers of the fine structure constant α

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

Leading relativistic correction

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

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

NRQED approach to few electron systems

Atomic energy levels are expanded in powers of the fine structure constant α

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

Leading QED correction

$$\begin{aligned} E^{(5)} \;=\; & \left[\frac{164}{15} + \frac{14}{3}\,\ln\alpha\right]\frac{\alpha^2}{m^2}\,\langle\delta^3(r_{12})\rangle \\ & + \left[\frac{19}{30} + \ln(Z\,\alpha)^{-2}\right]\frac{4\,\alpha^2\,Z}{3\,m^2}\,\langle\delta^3(r_1) + \delta^3(r_2)\rangle \\ & - \frac{14}{3}\,m\,\alpha^5\left\langle\frac{1}{4\,\pi}\,P\left(\frac{1}{(m\,\alpha\,r_{12})^3}\right)\right\rangle \\ & - \frac{2\,\alpha}{3\,\pi\,m^2}\left\langle\sum_a \vec{p}_a\,(H_0 - E_0)\,\ln\left[\frac{2\,(H_0 - E_0)}{(Z\,\alpha)^2\,m}\right]\sum_b \vec{p}_b\right\rangle \end{aligned}$$

NRQED approach to few electron systems

Atomic energy levels are expanded in powers of the fine structure constant α

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

Higher order effects $m\alpha^6$, $m\alpha^7 \cdots$

- $E^{(6)} = \langle H^{(6)} \rangle + \langle H^{(4)} \frac{1}{(E_0 - H_0)'} H^{(4)} \rangle$
- cancellation of singularities between the first and the second order matrix elements $\rightarrow$ difficult in numerical calculations
- $E^{(7)}$ known only for hydrogenic systems (+ He fs) $\rightarrow$ challenging task for few electron atoms

$2^3S - 2^3P$ transition in ^{4}He in MHz

	$(m/M)^0$	$(m/M)^1$	$(m/M)^2$	Sum
α^2	−276 775 637.536	102 903.459	−4.781	−276 672 738.857
α^4	−69 066.189	−6.769	−0.003	−69 072.961
α^5	5 234.163	−0.186	—	5 233.978
α^6	87.067	−0.029	—	87.039
α^7	−8.0 (1.0)	—	—	−8.0(1.0)
FNS	3.427	—	—	3.427
NPOL	−0.002	—	—	−0.002
Theory				−276 736 495.41 (1.00)
Exp.				−276 736 495.649 (2)

^{3}He - ^{4}He isotope shift of $2^3S - 2^3P$ centroid energies 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
Theory				33 667 149.3(0.9)

^{3}He - ^{4}He charge radii difference

$$\delta r^2(\text{Florence 2012}, 2^3P - 2^3S) = 1.069\,(3)\,\text{fm}^2\,,$$

$$\delta r^2(\text{Shiner 1995}, 2^3P - 2^3S) = 1.061\,(3)\,\text{fm}^2\,,$$

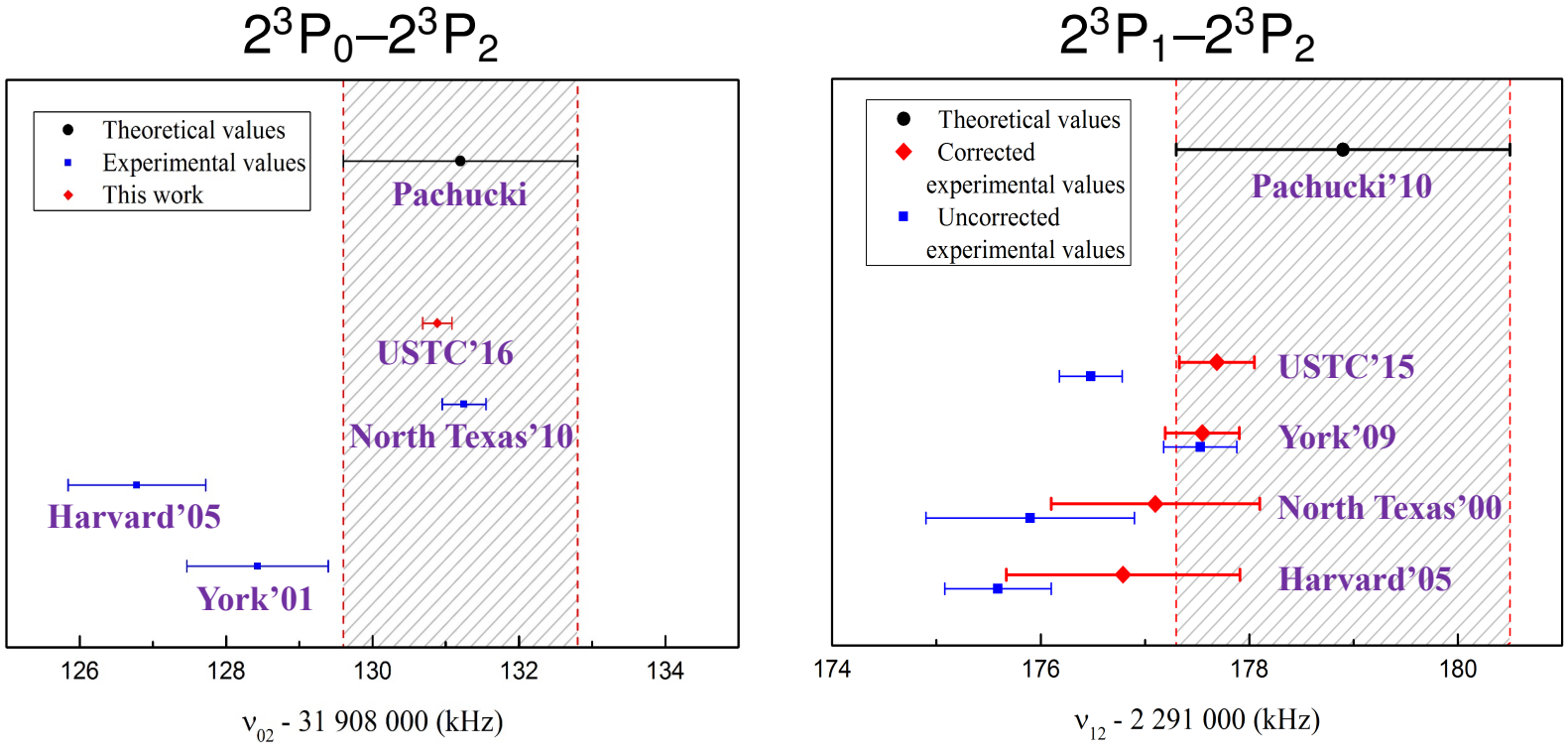
$$\delta r^2(\text{Amsterdam 2011}, 2^1S - 2^3S) = 1.028\,(11)\,\text{fm}^2$$

3.7 σ discrepancy

He fine structure

Term	ν_{01}	ν_{12}	Ref.
$m\alpha^4(+m/M)$	29 563 765.45	2 320 241.43	
	29 563 765.23	2 320 241.42	Drake (2002)
$m\alpha^5(+m/M)$	54 704.04	−22 544.00	
	54 704.04	−22 545.01	Drake (2002)
$m\alpha^6$	−1 607.52(2)	−6 506.43	
	−1 607.61(4)	−6 506.45(7)	Drake (2002)
$m\alpha^6 m/M$	−9.96	9.15	
	−10.37(5)	9.80(11)	Drake (2002)
$m\alpha^7 \log(Z\alpha)$	81.43	−5.87	
	81.42	−5.87	Drake (2002)
$m\alpha^7$, nlog	18.86	−14.38	
$m\alpha^8$	±1.7	±1.7	
Total theory	29 616 952.29 ± 1.7	2 291 178.91 ± 1.7	

Comparison with experiments: Yu Sun PSAS'16



Sensitive test of hypothetical additional long range interactions

Hydrogen molecule: comparison with experiment

H_2 has not been considered so far for high precision test of fundamental interactions

	D_0	$v = 0 \to 1$	$J = 0 \to 1$
$\alpha^2\, m$	36 118.797 746 12(5)	4 161.164 070 3(1)	118.485 260 46(3)
$\alpha^4\, m$	−0.531 8(3)[a]	0.023 41(1)[c]	0.002 580(1)
$\alpha^5\, m$	−0.194 8(2)[b]	−0.021 29(2)[c]	−0.001 022(1)
$\alpha^6\, m$	−0.002 065(6)	−0.000 192 3(6)	−0.000 008 9(1)
$\alpha^7\, m$	0.000 118(59)	0.000 012 0(60)	0.000 000 6(3)
$E_{r_p^2}$	−0.000 031	−0.000 003 2	−0.000 000 2
Theory	36 118.069 1(6)	4 161.166 01(4)	118.486 810(4)
Exp	36 118.069 62(37)	4 161.166 32(18)	118.486 84(10)

D_0 - dissociation energy in cm^{-1}

Dissociation energy – comparison with experiment

	D_0/cm^{-1}	
	H_2	D_2
Experiment (1993)[1]	36 118.06(4)	36 748.32(7)
Experiment (2004)[2]	36 118.062(10)	36 748.343(10)
Experiment (2009/10)[3,4]	36 118.069 62(37)	36 748.362 86(68)
Theory (2016), (2009)[5]	36 118.069 1(6)	36 748.363 4(9)
Difference	0.000 5(7)	0.000 5(11)

[1] E. E. Eyler, N. Melikechi, *Phys. Rev. A* **48**, R18 (1993);
[2] Y. Zang *et al.*, *Phys. Rev. Lett.* **92**, 203003 (2004);
[3] Liu, Salumbides, Hollenstein, Koelemeij, Eikema, Ubachs, Merkt, *JCP* **130**, 174306 (2009)
[4] Liu, Sprecher, Jungen, Ubachs, Merkt, *JCP* **132**, 154301 (2010);
[5] Piszczatowski, Lach, Przybytek, Komasa, Pachucki, Jeziorski, *JCTC* **5**, 3039 (2009)

Conclusions

The high accuracy achieved for few-electron atomic and molecular systems allows

- determination of the nuclear charge radii from experimental transition frequencies
- searching for any discrepancies with spectroscopic measurements and uncover unknown forces at the atomic scale
- low-energy tests of the Standard Model of fundamental interactions and of its various extensions

Collaborators

- J. Komasa, Poznań University
- M. Puchalski, Poznań University
- V. A. Yerokhin, St. Petersburg Technical University
- V. Patkóš, Charles University, Praga
- P. Czachorowski, PhD student, University of Warsaw
- G. Łach, University of Warsaw