Searching for BSM physics with light atomic systems

Krzysztof Pachucki

University of Warsaw

BSM in direct, indirect and tabletop experiments
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Motivation and challenges

- Measurements of transition frequencies can be very accurate, Garching 2010: $\nu(1S-2S)_{\mathrm{H}} = 2466\,061\,413\,187\,035(10)\ \mathrm{Hz}$
- simple atomic systems can be calculated very precisely, up to the nuclear structure corrections

The interface between the strong and electromagnetic interactions can be probed very accurately in light atomic systems

- how come r_p from (electronic) H differs by 4% from that of μH ?
- violation of lepton universality of SM ?
- incorrect Ry constant ?
  - 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 the project is to bring the high accuracy achieved for hydrogenic levels to few-electron atomic and molecular systems

- to search for any discrepancies with spectroscopic measurements and uncover unknown forces at the atomic scale
- determination of fundamental constants Ry, α. m_e
- for the determination of the nuclear charge radii from experimental transition frequencies and comparison with those obtained from the muonic atom spectroscopy

NRQED

$$
\begin{aligned}
H &= \frac{\vec{\pi}^2}{2\,m} + e\,A^0 - \frac{e}{2\,m}\,g\,\vec{s}\cdot\vec{B} - \frac{e}{4\,m^2}\,(g-1)\,\vec{s}\cdot\left(\vec{E}\times\vec{\pi} - \vec{\pi}\times\vec{E}\right) \\
&\quad - \frac{\vec{\pi}^4}{8\,m^3} - \frac{e}{6}\,r_E^2\,\nabla\cdot\vec{E} + \frac{e}{8\,m^3}\left[4\,\vec{\pi}^2\,\vec{s}\cdot\vec{B} + (g-2)\,\{\vec{\pi}\cdot\vec{B}\,,\,\vec{\pi}\cdot\vec{s}\}\right] \\
&\quad - \frac{e^2}{2}\,\alpha_E\,\vec{E}^2 - \frac{e^2}{2}\,\alpha_B\,\vec{B}^2 + \ldots
\end{aligned}
$$

- QED matching terms in $g, r_E^2, \alpha_E, \alpha_B$, and $\sim \delta^{(3)}(r_{ij})$
- The Feynman path approach is used to obtain the multi-electron propagator propagator $G(t-t')$, where t and t' are common to all *out* and *in* electrons respectively,

$$
G(E) = \frac{1}{E - H_0 - \Sigma(E)},
$$

Bound state energy level

$$G(E) = \frac{1}{E - H_0 - \Sigma(E)}$$

One considers the matrix element of $G(E)$ between the nonrelativistic wave function ϕ of a specified state

$$\begin{aligned}
\langle\phi|G(E)|\phi\rangle &= \frac{1}{E - E_0} + \frac{1}{(E - E_0)^2}\langle\phi|\Sigma(E)|\phi\rangle \\
&\quad + \frac{1}{(E - E_0)^2}\langle\phi|\Sigma(E)\frac{1}{E - H_0}\Sigma(E)|\phi\rangle + \ldots \\
&= \frac{1}{E - E_0 - \sigma(E)}
\end{aligned}$$

where

$$\sigma(E) = \langle\phi|\Sigma(E)|\phi\rangle + \langle\phi|\Sigma(E)\frac{1}{(E - H_0)'}\Sigma(E)|\phi\rangle + \ldots$$

The total binding energy E, namely the pole of the resolvent, is

$$E = E_0 + \sigma(E_0) + \sigma(E_0)\frac{\partial\sigma(E_0)}{\partial E_0} + \ldots$$

NRQED expansion

The basic assumption is that the binding energy can be expanded in powers of the fine structure constant α

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

and also in the electron nucleus mass ratio m/M.

NRQED expansion

The basic assumption is that the binding energy can be 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

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

Leading relativistic correction

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

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

NRQED expansion

The basic assumption is that the binding energy can be 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 expansion

The basic assumption is that the binding energy can be 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

He atom

- two electrons and a nucleus, $M/m = 7\,294.299\,541\,36(24)$
- $H = \frac{p_1^2}{2\,m} + \frac{p_2^2}{2\,m} - \frac{Z\,\alpha}{r_1} - \frac{Z\,\alpha}{r_2} + \frac{\alpha}{r_{12}} + \frac{(p_1+p_2)^2}{2\,M}$
- solution of the Schrödinger equation by the variational method

$$\phi = \sum_i c_i\, e^{-\alpha_i\, r_1 - \beta_i\, r_2 - \gamma_i\, r_{12}}$$

- nonelativistic energy can be calculated with an arbitrary numerical precision $\sim$ 40 digits

$2^3S - 2^3P$ 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.	[Florence.2004]			−276 736 495.649 5 (21)
Exp.	[Zheng.2017]			−276 736 495.600 0 (14)

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 $2^3S - 2^3P$

- $E(2^3S - 2^3P, ^4\mathrm{He})_{\mathrm{centroid}} = 276\,736\,495\,600.0(1.4)$ kHz, Zheng, 2017
- finite size effect: $E_{\mathrm{fs}} = 3\,427$ kHz
- since E_{fs} is proportional to r^2

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

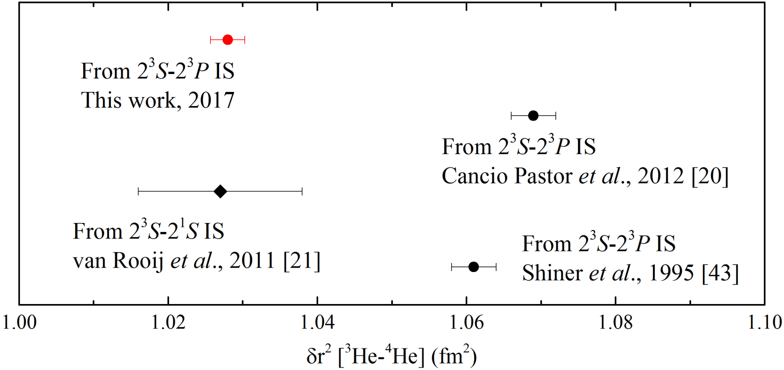
- electron scattering gives $r_{\mathrm{He}} = 1.681(4)$ fm, what corresponds to about $2.5 \cdot 10^{-3}$ relative accuracy
- $\sim$ 10 kHz accuracy requires calculation of $m\,\alpha^7$ correction

^{3}He - ^{4}He isotope shift of $2^3S - 2^3P$ in kHz

$E(^3\mathrm{He}, 2^3P - 2S)$ (centroid)	276 702 827 204.8 (2.4)
$-E(^4\mathrm{He}, 2^3P - 2S)$ (centroid)	−276 736 495 600.0 (1.4)
$-\delta E_{\mathrm{iso}}(2^3P - 2^3S)$ (point nucleus)	33 667 149.3 (0.9)
δE	−1 245.9 (2.9)
C	−1212.2 (1) $\mathrm{kHz/fm^2}$
δR^2	1.028 (2) $\mathrm{fm^2}$

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

$$
\begin{aligned}
\delta r^2(\text{Inguscio 2012}, 2^3P - 2^3S) &= 1.069\,(3)\,\mathrm{fm}^2\,, \\
\delta r^2(\text{Shiner 1995}, 2^3P - 2^3S) &= 1.061\,(3)\,\mathrm{fm}^2\,, \\
\delta r^2(\text{Vassen 2011}, 2^1S - 2^3S) &= 1.027\,(11)\,\mathrm{fm}^2 \\
\delta r^2(\text{Zheng 2017}, 2^1S - 2^3S) &= 1.028\,(11)\,\mathrm{fm}^2
\end{aligned}
$$


From 2^3S-2^3P IS
This work, 2017
From 2^3S-2^3P IS
Cancio Pastor *et al.*, 2012 [20]
From 2^3S-2^1S IS
van Rooij *et al.*, 2011 [21]
From 2^3S-2^3P IS
Shiner *et al.*, 1995 [43]
1.00
1.02
1.04
1.06
1.08
1.10
δr^2 [^{3}He-^{4}He] (fm^2)

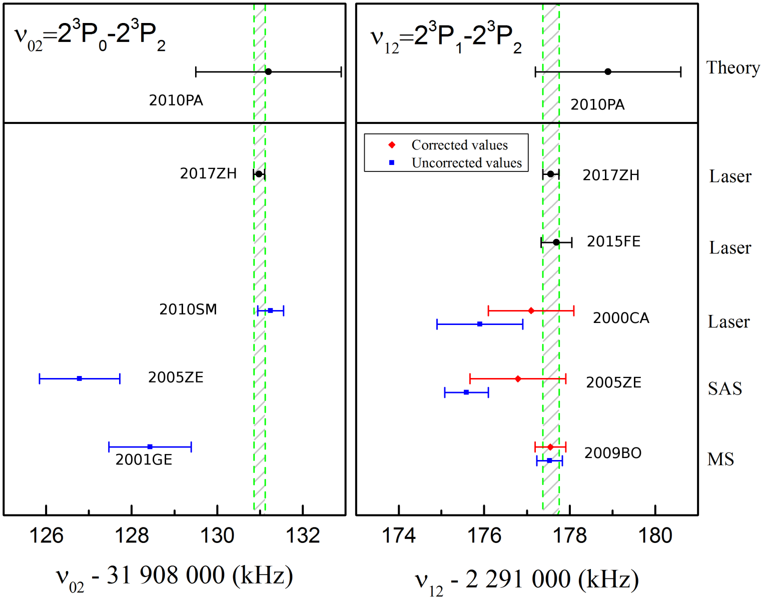
Comparison of exp. with theory for He transitions

	Theory	Experiment	
1^1S	5 945 204 173 (36)	5 945 204 212 (6)	Kandula (2011)
1^1S–2^1S	4 984 872 135 (36)	4 984 872 315 (48)	Bergeson (1998)
2^3S–3^3D_1	786 823 848.5 (2.6)[a]	786 823 850.002 (56)	Dorrer (1997)
2^3P_0–3^3D_1	510 059 753.7 (1.4)[a]	510 059 755.352 (28)	Luo (2016)
2^3P–2^3S	276 736 495.4 (1.0)[c]	276 736 495.649 (2)	Pastor (2004)[b]
2^3S–2^1P_1	338 133 594.0 (3.0)[c]	338 133 594.4 (5)	Notermans (2014)
2^1S–2^3S	192 510 703.4 (1.4)[c]	192 510 702.145 6 (18)	Rooij (2011)

[a] using theoretical value $E(3^3D_1) = 3\,660\,188\,92.97\,(2)$

[b] using theoretical results for 2^3P fine structure

Helium fine structure of 2^3P_J



Li atom

- three electrons and a nucleus, $M/m = 12789.39185475123$), ^{7}Li
- $H = \sum_i \left(\frac{p_i^2}{2\,m} - \frac{Z\,\alpha}{r_i}\right) + \sum_{i>j} \frac{\alpha}{r_{ij}} + \frac{(p_1+p_2+p_3)^2}{2\,M}$
- solution of the Schrödinger equation by the variational method

$$\begin{aligned}\psi &= \mathcal{A}[\phi(\vec{r}_1, \vec{r}_2, \vec{r}_3)\,\chi] \\ \phi &= \sum_{\{n\}} c_{\{n\}}\, e^{-\alpha r_1 - \beta r_2 - \gamma r_3}\, r_{23}^{n_1}\, r_{31}^{n_2}\, r_{12}^{n_3}\, r_1^{n_4}\, r_2^{n_5}\, r_3^{n_6} \\ \chi &= [\alpha(1)\,\beta(2) - \beta(1)\,\alpha(2)]\,\alpha(3)\end{aligned}$$

- calculation of integrals is highly nontrivial
- nonelativistic energy can be calculated with limited numerical precision $\sim$ 16 digits

^{6}Li-^{7}Li isotope shift and the charge radii diff.

$$\delta_{\rm fs} E = \frac{2\,\pi\,Z\,\alpha}{3}\,\left\langle\sum_a \delta^3(r_a)\right\rangle\,\langle r^2\rangle$$

$$\delta r^2 = r^2(^6\mathrm{Li}) - r^2(^7\mathrm{Li}) = \begin{cases} 0.705(3)\,\mathrm{fm}^2 \\ \qquad 2P_{1/2} - 2S_{1/2},\ \text{NIST (2013)} \\ \\ 0.700(9)\,\mathrm{fm}^2 \\ \qquad 2P_{3/2} - 2S_{1/2},\ \text{NIST (2013)} \\ \\ 0.731(22)\,\mathrm{fm}^2 \\ \qquad 3S_{1/2} - 2S_{1/2},\ \text{Nörtershäuser } \textit{et al} \text{ (2011)} \end{cases}$$

Li: ground state hyperfine structure

Fermi contact interaction

$$H_{\rm hfs} = \frac{2\,g_N\,Z\,\alpha}{3\,m\,M}\,\sum_a \vec{I}\cdot\vec{\sigma}_a\,\pi\,\delta^3(r_a)\,.$$

Finite nuclear size effect:

$$H_{\rm size} = -H_{\rm hfs}\,2\,Z\,\alpha\,m\,r_Z$$

where

$$r_Z = \int d^3r\,d^3r'\,\rho_E(r)\,\rho_M(r')\,|\vec{r}-\vec{r}'|$$

Li: hyperfine structure

	^{7}Li[MHz]	^{6}Li[MHz]
$A^{(4)}$	401.654 08(21)	152.083 69(11)
$A^{(5)}_{\mathrm{rec}}$	−0.004 14	−0.001 80
$A^{(6)}$	0.260 08(2)	0.098 48(1)
$A^{(7)}$	−0.010 2(13)	−0.003 9(5)
A_{the} (point nucleus)	401.899 8(13)	152.176 5(5)
A_{exp}	401.752 043 3(5)	152.136 839(2)
$(A_{\mathrm{exp}} - A_{\mathrm{the}})/A_{\mathrm{exp}}$	−368(3) ppm	−261(3) ppm
r_Z	3.25(3) fm	2.30(3) fm
r_E	2.390(30) fm	2.540(28) fm

significant dependence of r_Z on the isotope ?

Hydrogen molecule

- bound system of two electrons and two protons
- $H = \frac{p_A^2}{2\,M} + \frac{p_B^2}{2\,M} + \frac{p_1^2}{2\,m} + \frac{p_2^2}{2\,m} - \frac{\alpha}{r_{1A}} - \frac{\alpha}{r_{1B}} - \frac{\alpha}{r_{2A}} - \frac{\alpha}{r_{2B}} + \frac{\alpha}{r_{12}} + \frac{\alpha}{r_{AB}}$
- solved using the variational method

$$\Psi = \sum_{k=1}^{K} c_k\, \hat{S}\, \psi_{\{k\}}(\vec{r}_1, \vec{r}_2, \vec{R}_A, \vec{R}_B)$$

$$\psi_{\{k\}} = \exp\left[-\alpha\, r_{AB} - \beta\,(\zeta_1 + \zeta_2)\right] r_{AB}^{k_0}\, r_{12}^{k_1}\, \eta_1^{k_2}\, \eta_2^{k_3}\, \zeta_1^{k_4}\, \zeta_2^{k_5}\,,$$

where $\zeta_i = r_{iA} + r_{iB}$ and $\eta_i = r_{iA} - r_{iB}$

- Born-Oppenheimer approximation
  $\phi = \exp[-\alpha_1\, r_{1A} - \beta_1\, r_{1B} - \alpha_2\, r_{2A} - \beta_1\, r_{2B} - \gamma\, r_{12}]$
  implementation by M. Zientkiewicz and P. Czachorowski

Hydrogen molecule: comparison with experiment

D_0 - dissociation energy in cm^{-1}, corrections using BO approximation

	H_2	D_2
$\alpha^2\, m$	36 118.797 746 12(5)	36 749.090 98(8)
$\alpha^4\, m$	−0.531 121(1)	−0.529 170(1)
$\alpha^5\, m$	−0.194 8(2)	−0.198 2(2)
$\alpha^6\, m$	−0.002 067(6)	−0.002 096(6)
$\alpha^7\, m$	0.000 12(6)	0.000 12(6)
$E_{\rm fs}$	−0.000 031	−0.000 204
Theory	36 118.067 8(6)	36 748.361 4(4)
Exp	36 118.069 62(37)[a]	36 748.362 86(68)[b]
Difference	0.001 8	0.001 46

[a] Liu *et al.* (2009); [b] Liu *et al.* (2010)

for determination of r_p, Ry and for bounds on the long range interactions

r_p from dissociation energy of H_2

- $D_0(\mathrm{H}_2) = 36118.06962(37)\ \mathrm{cm}^{-1}$, J. Liu at al, 2009
- the proton charge radius which contributes $3.1\,10^{-5}\ \mathrm{cm}^{-1}$ to the dissociation energy
- at the $6 \cdot 10^{-7}\ \mathrm{cm}^{-1}$ accuracy for H_2 levels, r_p can be determined to 1.0% accuracy (discrepancy is at 4%)
- requires calculation of $m\,\alpha^7$ and the so called nonadiabatic corrections.
- significance of the uncertainties in the electron-proton mass ratio

Nuclear spin-spin coupling in HD

- The scalar nuclear spin-spin coupling $= J\, \vec{I}_A \cdot \vec{I}_B$
- this is a tiny effect $J \sim \alpha^6\, m^3/M^2$
- for the HD molecule $R_{AB} = 1.4$ au

$$J = \begin{cases} 43.115(9)\,\mathrm{Hz} & \text{Neronov 2014} \\ 43.12(1)\,\mathrm{Hz} & \text{Garbacz 2016} \\ 43.306(3)\,\mathrm{Hz} & \text{theory 2017} \end{cases}$$

- discrepancy is most probably caused by the adiabatic approximation
- J is the best probe of spin dependent BSM forces

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
- M. Zientkiewicz, PhD student, University of Warsaw