Bound-state QED calculations and the hydrogen molecular ion spectroscopy

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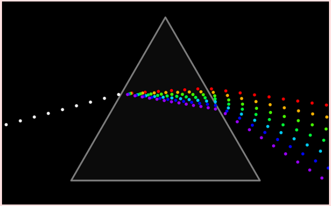

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Collaborators:

This work was done in collaboration with

- L. Hilico, J.-P. Karr, Laboratoire Kastler Brossel, UPMC-Univ. Paris 6, ENS, Paris, France
- J.C.J. Koelemeij, LaserLaB, VU University, Amsterdam, The Netherlands

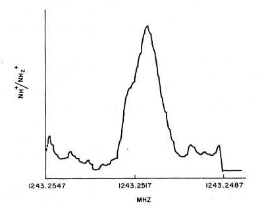
Outline:

- Hyperfine structure of H_2^+. Old problems and new results.
- Ro-vibrational spectroscopy of the H_2^+ and HD^+ molecular ions.
  - $m\alpha^7$ order contributions. Summary of recent numerical calculations.
  - $m\alpha^8$ order contributions. Present status.

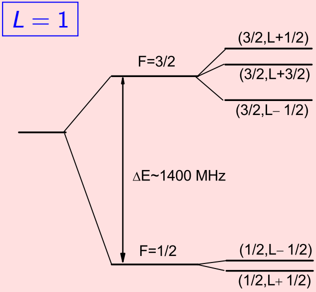
Hyperfine structure in H_2^+.

Hyperfine structure in H_2^+

Experiment by Jefferts:



Signal (effective photodissociation rate) versus frequency of applied rf magnetic field. [Jefferts, PRL **23**, 1476 (1969)].

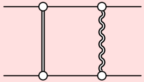


The effective Hamiltonian:

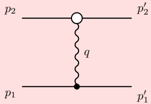
$$H_{\mathrm{eff}} = b_F(\mathbf{I}\cdot\mathbf{s}_e) + c_e(\mathbf{L}\cdot\mathbf{s}_e) + c_I(\mathbf{L}\cdot\mathbf{I}) + \frac{d_1}{(2L-1)(2L+3)}\left\{\frac{2}{3}\mathbf{L}^2(\mathbf{I}\cdot\mathbf{s}_e) - [(\mathbf{L}\cdot\mathbf{I})(\mathbf{L}\cdot\mathbf{s}_e)+(\mathbf{L}\cdot\mathbf{s}_e)(\mathbf{L}\cdot\mathbf{I})]\right\} + \frac{d_2}{(2L-1)(2L+3)}\left[\frac{1}{3}\mathbf{L}^2\mathbf{I}^2 - \frac{1}{2}(\mathbf{L}\cdot\mathbf{I}) - (\mathbf{L}\cdot\mathbf{I})^2\right].$$

NRQED contributions of order $(Z\alpha)^2 E_F$

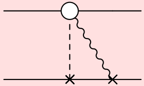
Second order term:



Higher order vertices:



Seagull interaction:



NRQED contributions of order $(Z\alpha)^2 E_F$

Second order term:

$$\Delta E_A = 2\alpha^4 \left\langle -\frac{\mathbf{p}_e^4}{8m_e^3} + \frac{Z}{8m_e^2}\,4\pi\left[\delta(\mathbf{r}_1)+\delta(\mathbf{r}_2)\right] \middle| Q(E_0-H_0)^{-1}Q \middle| \times \frac{8\pi}{3m_e}\,\mathbf{s}_e\left[\boldsymbol{\mu}_1\delta(\mathbf{r}_1)+\boldsymbol{\mu}_2\delta(\mathbf{r}_2)\right] \right\rangle$$

NRQED contributions of order $(Z\alpha)^2 E_F$

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Effective Hamiltonian $H^{(6)}$

The tree level interaction:

$$\mathcal{V}_1 = -e^2\left(\frac{[\boldsymbol{\sigma}_e^P\times\mathbf{q}](p_e'^2+p_e^2)}{8m_e^3}\right)\frac{1}{\mathbf{q}^2}\left(Z_i\frac{\boldsymbol{\sigma}_i^P\times\mathbf{q}}{2M_i}\right)$$

The seagull interaction with one Coulomb and one transverse photon lines:

$$\mathcal{V}_2 = e^4\frac{\boldsymbol{\sigma}_e^P}{4m_e^2}\left[\left\{\left[-\frac{1}{\mathbf{q}_2^2}\left(\delta^{ij}-\frac{q_2^iq_2^j}{\mathbf{q}_2^2}\right)\right]\left(-Z_2\frac{\mathbf{P}_2'+\mathbf{P}_2}{2M_2}\right)\right\}\times\left[\frac{i\mathbf{q}_1}{\mathbf{q}_1^2}\right](Z_1)\right]+(1\leftrightarrow2)$$

Radiative corrections

- Correction of order $\alpha(Z\alpha)E_F$:

$$E_r^{(6)} = \alpha^4 Z \left(\ln 2 - \frac{13}{4} + \frac{3}{4}\right) \frac{8\pi}{3m_e} \left\langle s_e \left[\boldsymbol{\mu}_1 \delta(\mathbf{r}_1) + \boldsymbol{\mu}_2 \delta(\mathbf{r}_2)\right] \right\rangle$$
$$= \alpha^2 \left[-96.2174 \cdot 10^{-6}\right] \frac{8\pi}{3m_e} \left\langle s_e \left[\boldsymbol{\mu}_1 \delta(\mathbf{r}_1) + \boldsymbol{\mu}_2 \delta(\mathbf{r}_2)\right] \right\rangle.$$

- Correction of order $\alpha(Z\alpha)^2 \ln^2(Z\alpha)E_F$

$$E_r^{(7)} = \alpha^5 Z^2 \left(-\frac{8}{3\pi}\right) \ln^2(Z\alpha) \frac{8\pi}{3m_e} \left\langle s_e \left[\boldsymbol{\mu}_1 \delta(\mathbf{r}_1) + \boldsymbol{\mu}_2 \delta(\mathbf{r}_2)\right] \right\rangle.$$

Corrections for the finite size of proton

- Zemach correction $((Z\alpha)(m/\Lambda)E_F)$:

$$E_Z = -\alpha^2 \frac{2r_Z}{a_0} \frac{8\pi}{3m_e} \left\langle s_e \boldsymbol{\mu}_p \delta(\mathbf{r}_p) \right\rangle = \alpha^2 \left[-40.08 \cdot 10^{-6}\right] \frac{8\pi}{3m_e} \left\langle s_e \boldsymbol{\mu}_p \delta(\mathbf{r}_p) \right\rangle$$

  where $r_Z = 1.045(16)$.

- Recoil correction of order $(Z\alpha)(m/M)E_F$:

$$E_{recoil} = \alpha^2 \left[5.48(6) \cdot 10^{-6}\right] \frac{8\pi}{3m_e} \left\langle s_e \boldsymbol{\mu}_p \delta(\mathbf{r}_p) \right\rangle$$

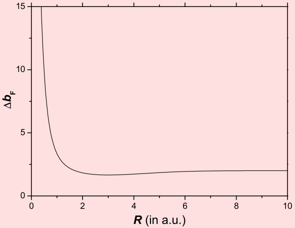
- Proton polarizability:

$$E_{pol} = \alpha^2 \left[1.4(6) \cdot 10^{-6}\right] \frac{8\pi}{3m_e} \left\langle s_e \boldsymbol{\mu}_p \delta(\mathbf{r}_p) \right\rangle$$

Hyperfine splitting of the hydrogen atom ground state

term	(kHz)
E_F	1418 840.096(9)
a_e	1 645.361
$(Z\alpha)^2$	113.333
$\alpha(Z\alpha)$	-136.517
$\alpha(Z\alpha)^2 \ln^2(Z\alpha)^{-1}$	-11.330
Higher order QED	1.23
proton structure (Zemach)	$-56.9(9)$
proton structure (recoil)	8.43(8)
proton structure (polarizability)	2.0(8)
$\Delta E(\mathrm{HFS})$	1420 405.7(1.7)
experiment	1420 405.751 7667(9)

Hyperfine splitting of the levels in H_2^+ vibrational states



$$\Delta E = 4\pi \int_0^\infty R^2 dR \left(\Delta b_F(R)\psi_0^2\right)$$

Effective potential of the Δb_F contribution of order $(Z\alpha)^2 E_F$

Table: Comparison of the spin-spin interaction coefficient b_F (in MHz) with experiment. $L = 1$. (Results of 2009.)

v	theory	experiment
4	836.720	836.729
5	819.219	819.227

Vibrational excitations

Let us reconsider the second order contribution:

$$\Delta E_A = 2\alpha^4 \left\langle H_B \left| Q(E_0 - H)^{-1} Q \right| H_{ss} \right\rangle$$

In the two-center approximation only the electron excitations are taken into this consideration.

In order to get the missing part, namely, the vibrational excitations, we should add to our analysis the third term:

$$\Delta E_B = 2\alpha^4 \sum_{v' \neq v} \frac{\langle vL|H_B|v'L\rangle \langle v'L|H_{ss}|vL\rangle}{E_v - E_{v'}}$$

where summation is carried out over the vibrational states of the $1s\sigma$ *electronic* state only.

Final results. Contributions

Table: A summary of contributions to the spin-spin interaction coefficient b_F (in MHz).

contribution	$v = 4$	$v = 5$	
b_F	836.7835	819.2801	
$(Z\alpha)^2$	0.0607	0.0596	
	0.0510	0.0511	old value
$\alpha(Z\alpha)$	−0.0804	−0.0787	
$\alpha(Z\alpha)^2 \ln^2(Z\alpha)$	−0.0067	−0.0065	
ΔE_Z	−0.0335(5)	−0.0328(5)	
ΔE_R^p	0.0049(1)	0.0045(1)	
$\Delta E_{\rm pol}$	0.0012(5)	0.0011(5)	
b_F(new)	836.7294(10)	819.2272(10)	

Final results

Table: Comparison of the spin-spin interaction coefficient b_F (in MHz) with experiment. $L = 1$.

v	old	new	experiment
4	836.720	836.7294	836.729
5	819.219	819.2272	819.227
6	803.167	803.1749	803.175
7	788.501	788.5077	788.508
8	775.166	775.1709	775.172

Ro-vibrational spectroscopy

Status of theory. H_2^+ and HD^+ ions

Fundamental transitions in H_2^+ and HD^+ (in MHz).
CODATA10 recommended values of constants.

	H_2^+	HD^+
ΔE_{nr}	65 687 511.0714	57 349 439.9733
ΔE_{α^2}	1091.0400	958.1514
ΔE_{α^3}	−276.5450	−242.1262
ΔE_{α^4}	−1.9969	−1.7481
ΔE_{α^5}	0.1372(1)	0.1201(1)
ΔE_{α^6}	−0.0017(5)	−0.0014(4)
ΔE_{tot}	65 688 323.7050(5)	57 350 154.3688(4)

The error bars in transition frequency set a limit on the fractional precision in determination of mass ratio to

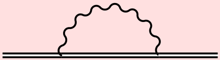
$$\frac{\Delta\mu}{\mu} = 1.5 \cdot 10^{-11}$$

RMS radius of proton

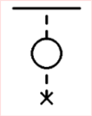
The proton rms charge radius uncertainty as is defined in the CODATA10 adjustment contributes to the fractional uncertainty at the level of $\sim 4 \cdot 10^{-12}$ for the transition frequency. While the muon hydrogen "charge radius" moves the spectral line blue shifted by 3 KHz that corresponds to a relative shift of $5 \cdot 10^{-11}$.

$m\alpha^7$ order contributions

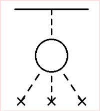
- One-loop self-energy



- One-loop vacuum polarization



- The Wichman-Kroll contribution



- Complete two-loop contribution
- Complete three-loop contribution

Summary of $m\alpha^7$ order contributions

Contributions of the $m\alpha^7$ order to the fundamental transitions in H_2^+ and HD^+ (in kHz).

	H_2^+	HD^+
ΔE_{1loop}	124.9(1)	109.3(1)
ΔE_{VP}	2.3	2.1
ΔE_{WK}	-0.1	-0.1
ΔE_{2loop}	10.1	8.7
ΔE_{3loop}	-0.06	-0.05
ΔE_{tot}	137.2(1)	120.1(1)

$m\alpha^8$ order contributions

Two-loop self-energy. Hydrogen.

The two-loop contribution at $m\alpha^8$ order for the hydrogen-like atom is

$$E^{(8)}_{2loop} = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^6}{n^3} \left[B_{63}\ln^3(Z\alpha)^{-2} + B_{62}\ln^2(Z\alpha)^{-2} + B_{61}\ln(Z\alpha)^{-2} + B_{60}\right]$$

For the ground state various contributions look like

$$\Delta E(1S) \approx \frac{\alpha^2(Z\alpha)^6}{\pi^2}\left[-282 - 62 + 476 - 61\right]$$

Two-loop self-energy

The coefficients B_{6k} may be calculated using expressions

$$Z^6 B_{63} = -\frac{8}{27} Z^3 \langle \pi\delta(\mathbf{r}) \rangle$$

$$Z^6 B_{62} = \frac{1}{9} \left\langle \boldsymbol{\nabla}^2 V\, Q(E_0 - H)^{-1} Q\, \boldsymbol{\nabla}^2 V \right\rangle_{\rm fin} + \frac{1}{18} \left\langle \boldsymbol{\nabla}^4 V \right\rangle_{\rm fin} + \frac{16}{9}\left[\frac{31}{15} + 2\ln 2\right] Z^3 \langle \pi\delta(\mathbf{r}) \rangle$$

The largest contribution (*for the hydrogen atom ground state*) is

$$Z^6 B_{61} = -2\left[\frac{1}{9} \left\langle \boldsymbol{\nabla}^2 V\, Q(E_0 - H)^{-1} Q\, \boldsymbol{\nabla}^2 V \right\rangle_{\rm fin} + \frac{1}{18} \left\langle \boldsymbol{\nabla}^4 V \right\rangle_{\rm fin}\right] \ln 2 + \frac{4}{3} N(n,l) + \frac{19}{135} \left\langle \boldsymbol{\nabla}^2 V\, Q(E_0 - H)^{-1} Q\, \boldsymbol{\nabla}^2 V \right\rangle_{\rm fin} + \frac{19}{270} \left\langle \boldsymbol{\nabla}^4 V \right\rangle_{\rm fin} + \frac{1}{24} \left\langle 2i\sigma^{ij} p^i \boldsymbol{\nabla}^2 V p^j \right\rangle + \left[\frac{48781}{64800} + \frac{2027\pi^2}{864} + \frac{56}{27}\ln 2 - \frac{2\pi^2}{3}\ln 2 + 8\ln^2 2 + \zeta(3)\right] Z^3 \langle \pi\delta(\mathbf{r}) \rangle$$

Low energy part $N(n,l)$

The low energy contribution $N(n,l)$ is defined

$$N = \frac{2}{3}\int_0^\Lambda k\,dk\;\delta_{\pi Z\delta(\mathbf{r})}\Big\langle \mathbf{p}(E_0-H-k)^{-1}\mathbf{p}\Big\rangle$$

where

$$\delta_{\pi Z\delta(\mathbf{r})}\Big\langle \mathbf{p}(E_0-H-k)^{-1}\mathbf{p}\Big\rangle \equiv$$

$$\Big\langle \mathbf{p}(E_0-H-k)^{-1}\Big(\pi\rho-\langle\pi\rho\rangle\Big)(E_0-H-k)^{-1}\mathbf{p}\Big\rangle$$

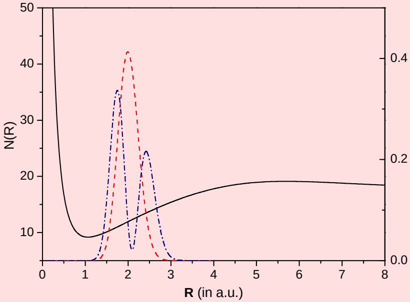
$$+2\Big\langle(\pi\rho)\;Q(E_0-H)Q\;\mathbf{p}(E_0-H-k)^{-1}\mathbf{p}\Big\rangle$$

Low energy part $N(n, l)$

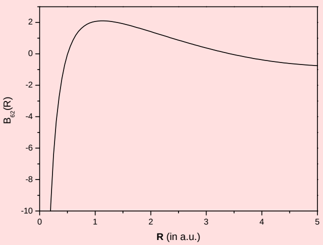
For the hydrogen ground state we got:

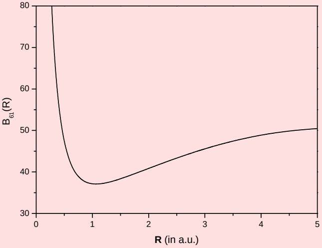
$$N(1S) = 17.8556720362(1).$$

For the two-center problem the effective potential of $N(R)$



Contributions $\alpha^2(Z\alpha)^6\ln^2(Z\alpha)$ and $\alpha^2(Z\alpha)^6\ln(Z\alpha)$





$$B_{62}\ \left\langle\pi\left(Z_1^3\delta(\mathbf{r}_1)+Z_2^3\delta(\mathbf{r}_2)\right)\right\rangle = 4\pi\int_0^\infty R^2dR\left(B_{62}(R)\psi_0^2\right)$$

$$B_{61}\ \left\langle\pi\left(Z_1^3\delta(\mathbf{r}_1)+Z_2^3\delta(\mathbf{r}_2)\right)\right\rangle = 4\pi\int_0^\infty R^2dR\left(B_{61}(R)\psi_0^2\right)$$

Results for the H_2^+ ion

For the ground state of H_2^+ (in kHz):

	B_{63}	B_{62}	B_{61}
ΔE	-37.0	17.3	27.3

For the fundamental transition $(L=0, v=0) \to (L'=0, v'=1)$ (in kHz):

	B_{63}	B_{62}	B_{61}
ΔE	0.97	-1.68	-0.51

One-loop self-energy

The one-loop contribution at $m\alpha^8$ order is expressed

$$E^{(8)}_{1loop} = \frac{\alpha}{\pi}\frac{(Z\alpha)^7}{n^3}\left[A_{71}\ln(Z\alpha)^{-2}+A_{70}\right]$$

Here

$$A_{71}(nS) = \pi\left[\frac{139}{64} - \ln 2\right]$$

The nonlogarithmic contribution A_{70} of order $m\alpha(Z\alpha)^7$ was never calculated directly. From the extrapolation of the $G_{se}(1S, Z\alpha)$ [Jentschura, Mohr, Soff, PRA **63** 042512 (2001)] one may get $A_{70} = 44.4$

Uehling potential

The one-loop contribution at $m\alpha^8$ order is expressed

$$E_{VP}^{(8)} = \frac{\alpha}{\pi}\frac{(Z\alpha)^7}{n^3}\left[V_{71}\ln(Z\alpha)^{-2} + V_{70}\right]$$

Here

$$V_{71}(nS) = \pi\frac{5}{96}$$

$$V_{70}(nS) = -\pi\frac{5}{48}\left(\psi(n+1) - \psi(1) - \ln n - \ln 2 - \frac{153}{80} - \frac{2}{n} + \frac{103}{48n^2}\right)$$

Summary of $m\alpha^8$ order contributions

Contributions of the $m\alpha^8$ order to the fundamental transitions in H_2^+ and HD^+ (in kHz).

	H_2^+	HD^+
ΔE_{2loop}	$-1.22(10)$	$-1.06(10)$
ΔE_{1loop}	$-0.97(30)$	$-0.85(30)$
ΔE_{VP}	-0.017	-0.015
ΔE_{tot}	$-2.2(3)$	$-1.9(3)$

Summary

- A new limit of precision for theoretical predictions is achieved. Relative uncertainty is now $7 \cdot 10^{-12}$ for *the hydrogen molecular ions* H_2^+ and HD^+.
- The proton rms charge radius uncertainty as is defined in the CODATA10 adjustment contributes to the fractional uncertainty at the level of $\sim 4 \cdot 10^{-12}$ for the transition frequency. While the muon hydrogen "charge radius" moves the spectral line blue shifted by 3 KHz that corresponds to a relative shift of $5 \cdot 10^{-11}$.
- The two-loop correction at the $m\alpha^8$ order is calculated (at least the three leading terms).
- The one-loop SE correction at the $m\alpha^8$ order is now the major uncertainty.

Thank you for your attention!