Ro-vibrational spectroscopy of the hydrogen molecular ion and antiprotonic helium

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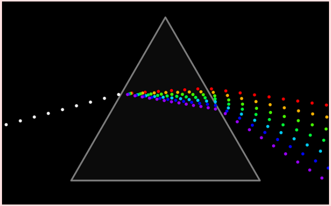


Fundamental Constants 2015, February 2015

Status of Theory. 2014

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}	0.1371(1)	0.1200(1)
ΔE_{α^6}	−0.0010(5)	−0.0009(4)
ΔE_{tot}	65 688 323.7055(5)	57 350 154.3693(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 $5 \cdot 10^{-11}$.

Antiprotonic helium

$$
\begin{aligned}
\Delta E_{nr} &= 2\,145\,088\,265.34 \\
\Delta E_{\alpha^2} &= -39\,349.33 \\
\Delta E_{\alpha^3} &= 5\,857.84 \\
\Delta E_{\alpha^4} &= 92.97 \\
\Delta E_{\alpha^5} &= -8.25(2) \\
\Delta E_{\alpha^6} &= -0.10(10) \\
\hline
\Delta E_{total} &= 2\,145\,054\,858.50(10)
\end{aligned}
$$

Transition $(33,32) \to (31,30)$ (in MHz).
CODATA10 recommended values of constants.

Along with the sensitivity of this transition to a change of $\mu \equiv m_{\bar{p}}/m_e$, this sets a limit on the fractional precision in determination of mass ratio

$$\boxed{\frac{\Delta\mu}{\mu} = 3.6 \cdot 10^{-11}}$$

Atomic mass of electron $A_r(e)$

At present the most precise measurements of m_p/m_e are:

The penning trap mass spectroscopy (uncertainty 2.1×10^{-9})
[D.L. Farnham, *et al.* Phys. Rev. Lett. **75**, 3598 (1995)];

The g factor of a bound electron in $^{12}C^{5+}$ (uncertainty 5.2×10^{-10})
[T. Beier, *et al.* Phys. Rev. Lett. **88**, 011603 (2001) and CODATA-10].

The spin-flip energy for a free electron is

$$\Delta E = -g_e \mu_B B$$

The analogous expression for ions with no nuclear spin

$$\Delta E = -g_e(X) \mu_B B$$

where the theoretical expression for $g_e(X)$ is written as

$$g_e(X) = g_D + \Delta g_{\rm rad} + \Delta g_{\rm rec} + \Delta g_{\rm ns} + \dots$$

g_D is derived from the Dirac equation

$$g_D = -\frac{2}{3}\left[1 + 2\sqrt{1-(Z\alpha)^2}\right] = -2\left[1 - \frac{1}{3}(Z\alpha)^2 + \dots\right]$$

Theoretical uncertainty of the g factor for $^{12}C^{5+}$ is $\boxed{1.3 \times 10^{-11}}$

High–precision measurement of the atomic mass of the electron

S. Sturm[1], F. Köhler[1,2], J. Zatorski[1], A. Wagner[1], Z. Harman[1,3], G. Werth[4], W. Quint[2], C. H. Keitel[1] & K. Blaum[1]

Nature, **506**, 467 (2014)

"Here we combine a very precise measurement of the magnetic moment of a single electron bound to a carbon nucleus with a state-of-the-art calculation in the framework of bound-state quantum electrodynamics. The precision of the resulting value for the atomic mass of the electron surpasses the current literature value of the Committee on Data for Science and Technology (CODATA) by a factor of 13."

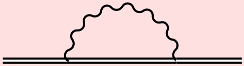
$$m_e = 0.000548579909067(14)(9)(2) \quad [3\times 10^{-11}]$$

$m\alpha^7$ order contributions

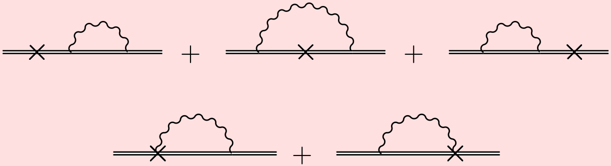
One-loop SE corrections in order $m\alpha^7$

1. One-loop SE corrections in order $m\alpha^7$

Main diagram:



Contributions at order $m\alpha^7$:



1. One-loop SE correction in atomic units

We rederived the low-energy part [V.I. Korobov, J.-P. Karr, and L. Hilico, Phys. Rev, A **89**, 032511 (2014)], and obtained an expression in atomic units, which may be extended for a general case of two and more external Coulomb sources:

$$\Delta E^{(7)}_{\rm se} = \frac{\alpha^5}{\pi}\Bigg\{\mathcal{L}(Z,n,l) + \left(\frac{5}{9}+\frac{2}{3}\ln\left[\frac{1}{2}\alpha^{-2}\right]\right)\left\langle 4\pi\rho\, Q(E-H)^{-1}Q\, H_B\right\rangle_{\rm fin_{au}}$$
$$+2\left\langle H_{so}\, Q(E-H)^{-1}Q\, H_B\right\rangle + \left(\frac{779}{14400}+\frac{11}{120}\ln\left[\frac{1}{2}\alpha^{-2}\right]\right)\left\langle \boldsymbol{\nabla}^4 V\right\rangle_{\rm fin_{au}}$$
$$+\left(\frac{23}{576}+\frac{1}{24}\ln\left[\frac{1}{2}\alpha^{-2}\right]\right)\left\langle 2i\sigma^{ij}p^i\boldsymbol{\nabla}^2 V p^j\right\rangle$$
$$+\left(\frac{589}{720}+\frac{2}{3}\ln\left[\frac{1}{2}\alpha^{-2}\right]\right)\left\langle (\boldsymbol{\nabla} V)^2\right\rangle_{\rm fin_{au}} + \frac{3}{80}\left\langle 4\pi\rho\,\mathbf{p}^2\right\rangle_{\rm fin_{au}} - \frac{1}{4}\left\langle \mathbf{p}^2 H_{so}\right\rangle$$
$$+Z^2\left[-\ln^2\left[\alpha^{-2}\right]+\left[\frac{16}{3}\ln 2-\frac{1}{4}\right]\ln\left[\alpha^{-2}\right]-0.81971202(1)\right]\langle\pi\rho\rangle\Bigg\}$$

1. Relativistic corrections to BL. Antiprotonic Helium

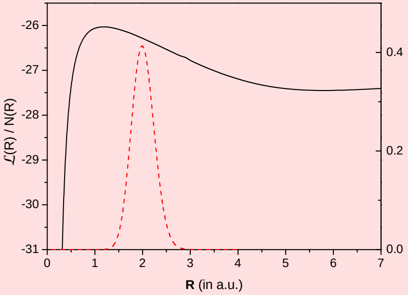
Relativistic Bethe logarithm for the ground electronic state. 2013.

R	$\beta_1^{(a)}$	$\beta_1^{(b)}$	β_2	β_3
0.1	−137.1	329.2	−102.	−381.08
0.2	−181.5	211.2	−584.1	62.514
0.4	−193.8	160.65	−1382.7	369.822
0.6	−241.21	150.07	−2064.5	590.636
1.0	−304.14	172.37	−2860.8	840.902

Relativistic Bethe logarithm for the ground electronic state. 2014.

R	$\beta_1^{(a)}$	$\beta_1^{(b)}$	β_2	β_3
0.05	−625.8(8)	650.5(5)	1797.(2)	−1486.18(2)
0.1	−291.5(1)	330.9(2)	177.1(6)	−381.72(3)
0.2	−181.68(4)	208.76(3)	−588.20(4)	63.099(5)
0.4	−194.00(1)	161.76(3)	−1387.92(5)	369.680(5)
0.6	−241.296(4)	151.068(3)	−2069.932(3)	590.555(2)
1.0	−304.531(3)	172.282(2)	−2862.089(1)	840.862(3)

1. Relativistic corrections to the Bethe logarithm



The relativistic Bethe logarithm $\mathcal{L}(R)$ for the ground $(1s\sigma_g)$ electronic state, for $Z_1 = Z_2 = 1$ normalized by: $N(R) = \pi\left(Z_1^3\delta(\mathbf{r}_1) + Z_2^3\delta(\mathbf{r}_2)\right)$.
[PRA **87**, 062506 (2013)]

Hydrogen molecular ion:

$$E^{(7)}_{1loop-se} = \alpha^5\left[A_{62}\ln^2(\alpha^{-2}) + A_{61}\ln(\alpha^{-2}) + A_{60}\right]\left\langle Z_1^3\delta(\mathbf{r}_1) + Z_2^3\delta(\mathbf{r}_2)\right\rangle \approx 124.9(1)\ \text{kHz},$$

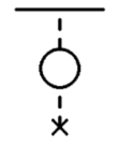
Other contributions beyond the self-energy

2. One-loop vacuum polarization

$$\Delta E_{1loop-vp} = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}\left\{V_{40}+(Z\alpha)V_{50}+(Z\alpha)^2V_{61}\ln(Z\alpha)^{-2}+\dots\right\}$$

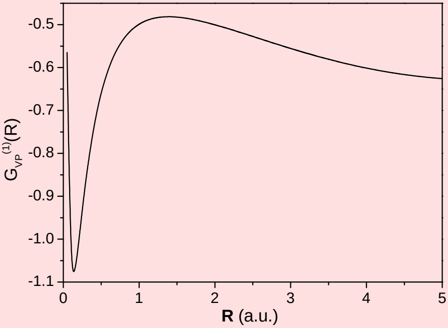
For the hydrogen atom in S-state the coefficients are

$$\begin{cases} V_{40}(nS) = -\dfrac{4}{15} \\ V_{50}(nS) = \pi\dfrac{5}{48} \\ V_{61}(nS) = -\dfrac{2}{15}, \\ V_{60}(nS) = \dfrac{4}{15}\left[-\dfrac{431}{105}+\psi(n+1)-\psi(1)-\dfrac{2(n-1)}{n^2}+\dfrac{1}{28n^2}-\ln\dfrac{n}{2}\right], \end{cases}$$



2. One-loop vacuum polarization

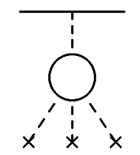
"Effective" potential for the H_2^+ ion at $m\alpha^7$ order including higher orders.



Hydrogen molecular ion:

$$E^{(7)}_{1loop-vp} = \alpha^5 \left[V_{61} \ln(\alpha^{-2}) + V_{60} \right] \left\langle Z_1^3 \delta(\mathbf{r}_1) + Z_2^3 \delta(\mathbf{r}_2) \right\rangle \approx 2.9 \text{ kHz},$$

3. The Wichman-Kroll contribution



$$\Delta E_{WK} = \frac{\alpha}{\pi}\frac{(Z\alpha)^6}{n^3}\left\{W_{60} + (Z\alpha)W_{70} + \dots\right\}$$

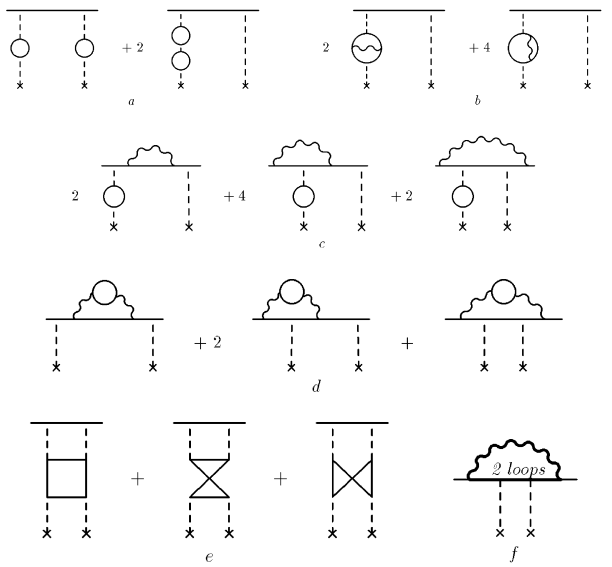
For the hydrogen atom in S-state the coefficients are

$$\begin{cases} W_{60}(nS) = \dfrac{19}{45} - \dfrac{\pi^2}{27}, \\ W_{70}(nS) = \dfrac{\pi}{16} - \dfrac{31\pi^3}{2880} \end{cases}$$

Hydrogen molecular ion:

$$E_{WK}^{(7)} = \alpha^5 W_{60}\left\langle Z_1^3\delta(\mathbf{r}_1) + Z_2^3\delta(\mathbf{r}_2)\right\rangle \approx -0.1\ \text{kHz},$$

4. Complete two-loop contribution



4. Complete two-loop contribution

$$\Delta E_{2loop} = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^4}{n^3}\left[B_{40} + (Z\alpha)B_{50} + \dots\right]$$

Here $B_{50} = -21.55447(13)$.

N.B. Insertion of two radiative photons in the electron line contributes $-24.269\dots$ to B_{50}

Hydrogen molecular ion:

$$E^{(7)}_{2loop} = \frac{\alpha^5}{\pi}\,[B_{50}]\left\langle Z_1^2\delta(\mathbf{r}_1)+Z_2^2\delta(\mathbf{r}_2)\right\rangle \approx 10.1\ \text{kHz},$$

5. Three-loop contribution

Three-loop contribution

$$\Delta E_{3loop} = \left(\frac{\alpha}{\pi}\right)^3 \frac{(Z\alpha)^4}{n^3}\left[0.417504 + \dots\right]$$

is already negligible.

Hydrogen molecular ion:

$$E^{(7)}_{3loop} = \frac{\alpha^5}{\pi^2}\,[0.417504]\,\langle Z_1\delta(\mathbf{r}_1)+Z_2\delta(\mathbf{r}_2)\rangle \approx 60\ \text{Hz},$$

Prospects for the future
$m\alpha^8$ order contributions

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.

Hydrogen molecular ion:

$$E^{(8)}_{1loop-se} = \frac{\alpha^6}{\pi}\left[A_{71}\ln(Z\alpha)^{-2} + A_{70}\right]\left\langle Z_1^4\delta(\mathbf{r}_1) + Z_2^4\delta(\mathbf{r}_2)\right\rangle \approx -0.5 \text{ kHz},$$

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

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

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

Hydrogen molecular ion:

$$E_{1loop-vp}^{(8)} = \frac{\alpha^6}{\pi}\left[V_{71}\ln(Z\alpha)^{-2} + V_{70}\right]\left\langle Z_1^4\delta(\mathbf{r}_1) + Z_2^4\delta(\mathbf{r}_2)\right\rangle \approx -17\text{ Hz},$$

Wichman-Kroll contribution

The Wichman-Kroll contribution at $m\alpha^8$ order

$$E_{WK}^{(8)} = \frac{\alpha}{\pi}\frac{(Z\alpha)^7}{n^3}\left[\frac{\pi}{16} - \frac{31\pi^3}{2880}\right]$$

Two-loop self-energy

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

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

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

Hydrogen molecular ion:

$$E^{(8)}_{2loop-vp} = \frac{\alpha^6}{\pi}\Big[B_{73}\ln^3(Z\alpha)^{-2} + B_{72}\ln^2(Z\alpha)^{-2} + B_{71}\ln(Z\alpha)^{-2} + B_{70}\Big]\left\langle Z_1^3\delta(\mathbf{r}_1) + Z_2^3\delta(\mathbf{r}_2)\right\rangle \approx -0.5\ \text{kHz},$$

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

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

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

The largest contribution is

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

Low energy part $N(n,l)$

The only quantity that needs numerical computations is $N(n,l)$, and it is defined by

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

and

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

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

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

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^+, and about $4.7 \cdot 10^{-11}$ for *the antiprotonic helium*.
- 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 become now the major uncertainty in the theory.
- The two-loop SE correction at the $m\alpha^8$ order is now under consideration and we hope to get the results by the end of this year. That should allow to improve theoretical uncertainty by a factor of 3-5.

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