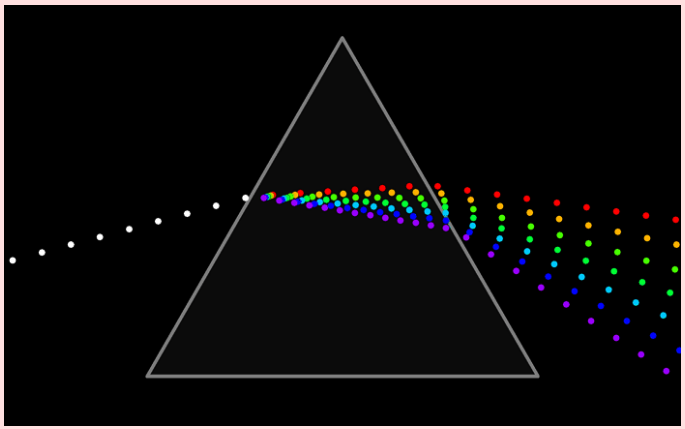
Precision spectroscopy of hydrogen molecular ions: present status of theory and perspectives

V.I. Korobov
Joint Institute for Nuclear Research
141980, Dubna, Russia
korobov@theor.jinr.ru



PSAS, Vienna, May 15, 2018

NRQED energy expansion

Physical energies (frequencies) are calculated in the NRQED formalism:

$$E(\alpha,\beta) = E_0 + \alpha^2 E_{rel} + \alpha^3 E^{(3)}_{\rm QED} + \alpha^4 E^{(4)}_{\rm QED} + \dots$$
$$+ \alpha^2 E^{(fs)}_{rel} + \alpha^3 \beta E^{(3)}_{\rm QED\ rec}$$
$$\vdots$$

Here:
$\alpha \approx 1/137$ — fine structure constant,
$\beta = m_e/M \sim 10^{-3}$ — electron-nuclear mass ratio.

Pure rotational transition $(L = 0, v = 0) \to (1, 0)$ in HD^+

Pure rotational transition in HD^+ (in kHz).
CODATA14 recommended values of constants.

	HD^+
ΔE_{nr}	1 314 886 776.354
ΔE_{α^2}	48 416.164
ΔE_{α^3}	−9 378.125
ΔE_{α^4}	−65.625(2)
ΔE_{α^5}	3.923(3)
ΔE_{α^6}	−0.070(18)
ΔE_{tot}	1 314 925 752.627(18)

$$u_r(\nu) = u_r(\mu) = 1.35 \times 10^{-11}$$

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 $A_{70} = 44.4$

Two-loop self energy at $m\alpha^8$

For the *fundamental rotational transition* $(L=0, v=0) \to (1,0)$ (in Hz)

$$\Delta\nu^{(8)}_{2loop} = \alpha^6 \left[B^{\nu}_{63} L^3(\alpha) + B^{\nu}_{62} L^2(\alpha) + B^{\nu}_{61} L(\alpha) + B^{\nu}_{60}\right]$$
$$\approx 32.8 - 43.3 - 33.9 + 7.1,$$

and for the uncertainty we take $u_r(E_{2loop}) = 7.1$ Hz.

Summary of $m\alpha^8$ order contributions

Contributions of the $m\alpha^8$ order to the fundamental rotational transition in HD^+ (in Hz).

	HD^+
$\Delta E_{1loop-SE}$	$-33.1(16.3)$
ΔE_{VP}	-0.59
ΔE_{2loop}	$-37.2(7.1)$
ΔE_{tot}	$-70.3(17.5)$

Other transitions in HD^+

Other transitions in HD^+ (in kHz).
CODATA14 recommended values of constants.

	HD^+	$u_r(\nu)$
$(0,0) \to (0,1)$	57 350 154 373.4(5)	7.9×10^{-12}
$(0,0) \to (1,1)$	58 605 052 157.5(5)	8.1×10^{-12}
$(2,0) \to (3,4)$	214 978 560 967.8(1.5)	7.8×10^{-12}
$(2,0) \to (3,8)$	383 407 177 209.4(2.9)	7.6×10^{-12}
$(3,0) \to (3,9)$	415 264 925 466.6(3.1)	7.5×10^{-12}

Rydberg constant

The new theoretical relative uncertainty for the fundamental transition frequency in H_2^+ is $u_r(\nu(H_2^+)) = 7.6 \times 10^{-12}$. For the ionization energy: $u_r(E_I) = 4.5 \times 10^{-12}$.

The CODATA14 uncertainty of the Rydberg constant is $u_r(R_\infty) = 5.9 \times 10^{-12}$.

Since this constant enters in the transition frequency $\nu(H_2^+)$ as a multiplier, a relative uncertainty *from the HMI spectroscopy* should be equal to $u_r(R_\infty) = u_r(\nu(H_2^+)) = 7.6 \times 10^{-12}$.

RMS radius of proton

The proton rms charge radius uncertainty as is defined in the CODATA14 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 $5 \cdot 10^{-11}$.

In case if we use the *"muon hydrogen" adjusted Rydberg constant* along with the *muon charge radius* then we get a shift of 1.1 kHz, which is still feasible for detection.

Precision spectroscopy of the hydrogen molecular ions H_2^+ and/or HD^+ allows to discriminate the "muon" charge radius and the CODATA value.

Master equation

To be used for adjustment of the fundamental constants, the frequency dependence of transition lines on the Rydberg constant, masses and proton charge radius may be expressed:

$$\nu(\mathrm{H}_2^+) = \nu_0(\mathrm{H}_2^+) + \frac{\Delta R_\infty}{R_\infty}\,\nu_0(\mathrm{H}_2^+) + 2(R_\infty c)\times \left[-2.55528\cdot 10^{-6}\Delta\mu_p - 8.117\cdot 10^{-12}\Delta r_p\right]$$

$\Delta R_\infty = R_\infty - R_{\infty,0}$, $\Delta\mu_p = \mu_p - \mu_{p,0}$ and $\Delta r_p = r_p^2 - r_{p,0}^2$.

Here the subscript 0 stands for the CODATA14 value, and ν_0 is the transition frequency presented in the final table.

Proton-to-electron mass ratio

The theoretical uncertainty on the fundamental transition in H_2^+ sets the limit on the achievable precision of the proton-to-electron mass ratio ($\mu = m_p/m_e$) to

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

This uncertainty is smaller by a factor of 6 with respect to the present CODATA14, $u_r(\mu_p) = 9.5 \times 10^{-11}$, which is currently limited by uncertainty on the proton's atomic mass.

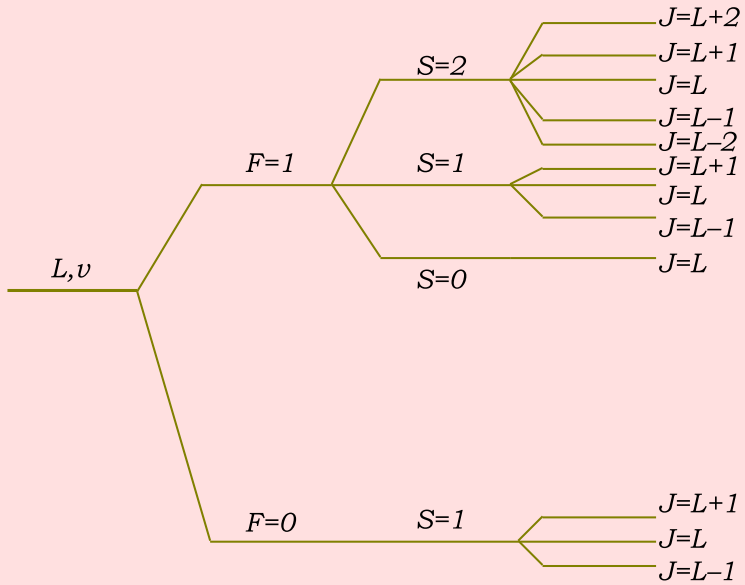
The electron's atomic mass has been recently improved ($u_r(A_r(e)) = 3.1 \times 10^{-11}$) by a high-precision measurement of the g-factor of a bound electron in a $^{12}C^{5+}$ ion.

HFS and spin-dependent part of transitions

HFS of HD^+ molecular ion

Coupling scheme:

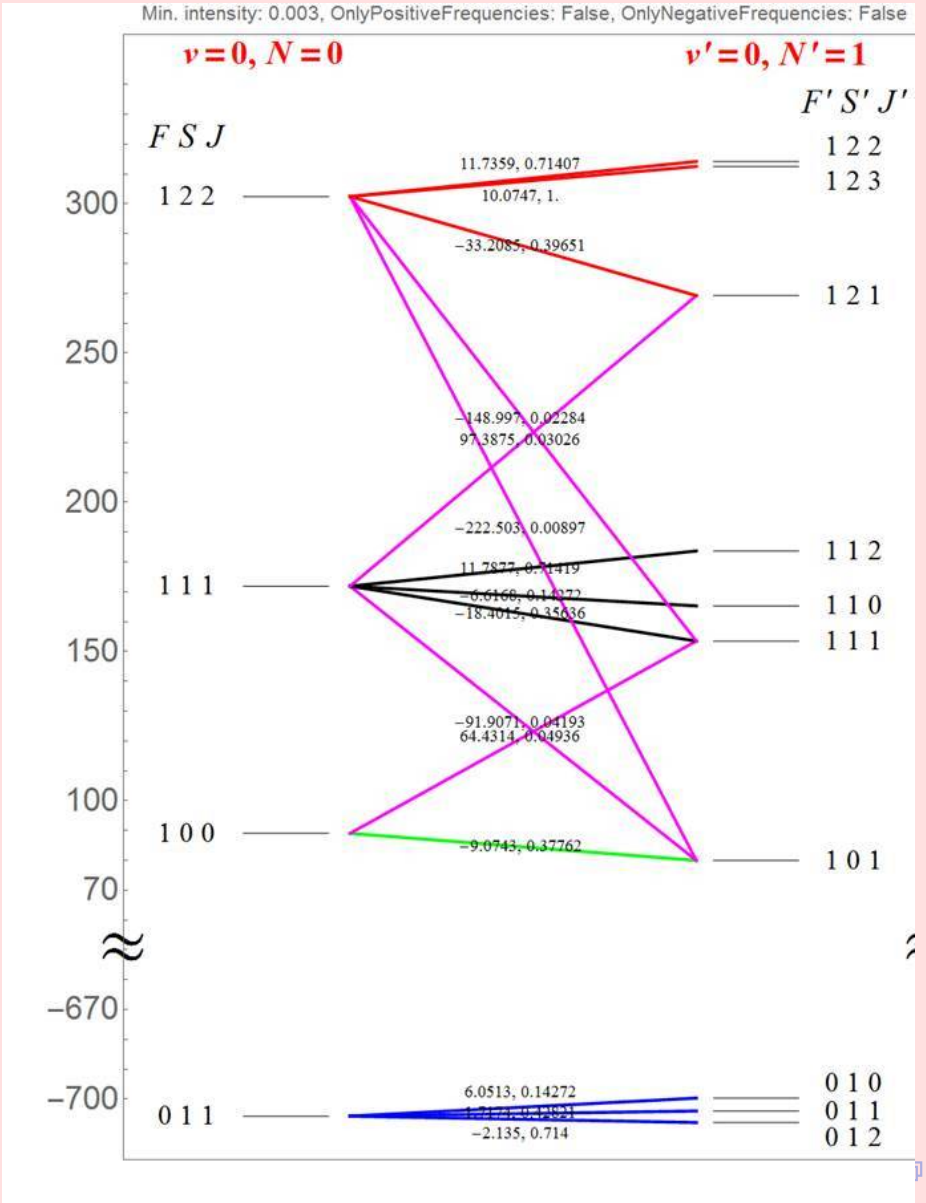
$$\begin{cases} \mathbf{F} = \mathbf{I}_p + \mathbf{s}_e, \\ \mathbf{S} = \mathbf{F} + \mathbf{I}_d, \\ \mathbf{J} = \mathbf{S} + \mathbf{L}. \end{cases}$$



Effective Hamiltonian:

$$\begin{aligned} H_{\rm HFS} = {} & E_1(\mathbf{L}\cdot\mathbf{s}_e) + E_2(\mathbf{L}\cdot\mathbf{I}_p) + E_3(\mathbf{L}\cdot\mathbf{I}_d) + E_4(\mathbf{I}_p\cdot\mathbf{s}_e) + E_5(\mathbf{I}_d\cdot\mathbf{s}_e) \\ & + E_6\Big\{2\mathbf{L}^2(\mathbf{I}_p\cdot\mathbf{s}_e) - 3[(\mathbf{L}\cdot\mathbf{I}_p)(\mathbf{L}\cdot\mathbf{s}_e) + (\mathbf{L}\cdot\mathbf{s}_e)(\mathbf{L}\cdot\mathbf{I}_p)]\Big\} \\ & + E_7\Big\{2\mathbf{L}^2(\mathbf{I}_d\cdot\mathbf{s}_e) - 3[(\mathbf{L}\cdot\mathbf{I}_d)(\mathbf{L}\cdot\mathbf{s}_e) + (\mathbf{L}\cdot\mathbf{s}_e)(\mathbf{L}\cdot\mathbf{I}_d)]\Big\} \\ & + E_8\Big\{2\mathbf{L}^2(\mathbf{I}_p\cdot\mathbf{I}_d) - 3[(\mathbf{L}\cdot\mathbf{I}_p)(\mathbf{L}\cdot\mathbf{I}_d) + (\mathbf{L}\cdot\mathbf{I}_d)(\mathbf{L}\cdot\mathbf{I}_p)]\Big\} \\ & + E_9\left[\mathbf{L}^2\mathbf{I}_d^2 - \frac{3}{2}(\mathbf{L}\cdot\mathbf{I}_d) - 3(\mathbf{L}\cdot\mathbf{I}_d)^2\right]. \end{aligned}$$

HF Structure of the fundamental rotational transition



Theory for stretch states

Spin-averaged transition frequency:

$$f_{\mathrm{spin-avg}} = 1\,314\,925.752\,627(18)\ \mathrm{MHz}$$

Hyperfine shift:

$$\begin{aligned}\Delta E(vL(F=1,S=2,J=L+2,m_J=\pm J))/h &= E_4/4 + E_5/2 \\ &+(E_1+E_2+2E_3+E_6+2E_7+2E_8+E_9)\,L/2 \\ &-(2E_6+4E_7+4E_8+2E_9)\,L^2/2 \\ &= 10.0747(10)\ \mathrm{MHz},\end{aligned}$$

So far, the coefficients have been calculated within the BreitPauli approximation.

HFS transition rates

The transition probability per time unit for states $E_i > E_f$ for an $E1$ transition is expressed

$$A_{i\to f} = \frac{4\alpha^3}{3\tau_0}(E_i - E_f)^3 \frac{|\langle i\, L_i \|\mathbf{d}\| f\, L_f\rangle|^2}{2L_i+1}$$

where $\tau_0 \approx 2.4189 \times 10^{-17}$ s is the unit of time in atomic units.

For the fundamental rotational transition: $A_{i\to f} = 0.669 \times 10^{-2}$ s^{-1}, or the life-time of the excited $(L = 1, v = 0)$ state is about 150 seconds.

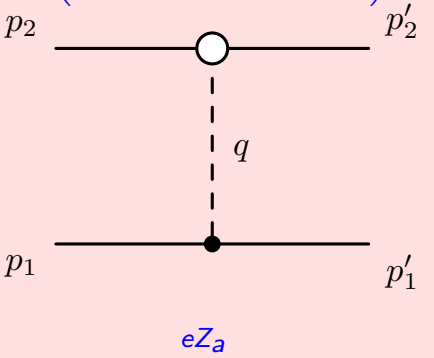
Taking into account spins one gets:

$$A_{i,FSJ\to f,F'S'J'} = (2J+1)(2J'+1)\begin{Bmatrix} L & 1 & L' \\ J' & S & J \end{Bmatrix}^2 A_{i\to f}$$

Future perspectives

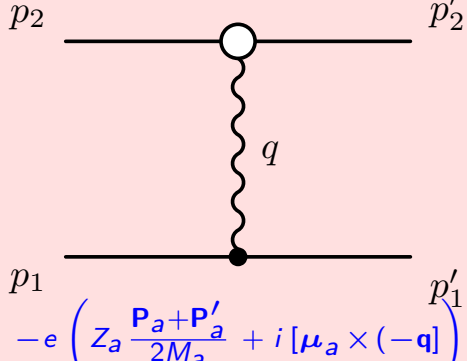
NRQED Feynman diagrams at order $m(Z\alpha)^6$

$$-e\left(\frac{3\mathbf{q}^2(p_e'^2+p_e^2)}{64m^4}+\frac{5(p'^2-p^2)^2}{128m^4}\right)$$
$$+e\,i\left(\frac{3\boldsymbol{\sigma}_e^P[\mathbf{q}\times\mathbf{p}_e](p_e'^2+p_e^2)}{32m^4}\right)$$



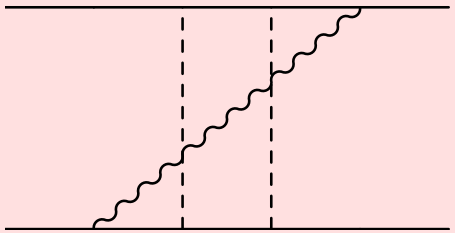
eZ_a

$$-e\left(\frac{\mathbf{p}_e'(3p_e'^2+p_e^2)+\mathbf{p}_e(3p_e^2+p_e'^2)}{16m^3}\right)$$
$$-e\,i\left(\frac{[\boldsymbol{\sigma}_e^P\times\mathbf{p}_e'](3p_e'^2+p_e^2)-[\boldsymbol{\sigma}_e^P\times\mathbf{p}_e](3p_e^2+p_e'^2)}{16m^3}\right)$$



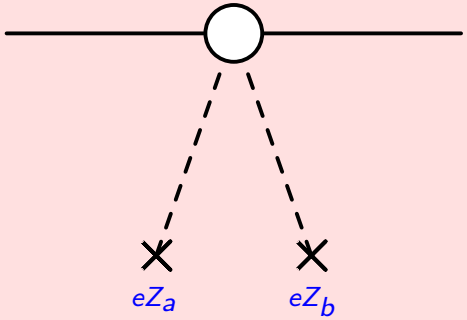
$$-e\left(Z_a\frac{\mathbf{P}_a+\mathbf{P}_a'}{2M_a}+i\,[\boldsymbol{\mu}_a\times(-\mathbf{q}]\right)$$

$$e\left(\frac{\mathbf{p}_e'+\mathbf{p}_e}{2m_e}+i\,\frac{\boldsymbol{\sigma}_e^P[\mathbf{q}\times\mathbf{p}_e]}{2m_e}\right)$$

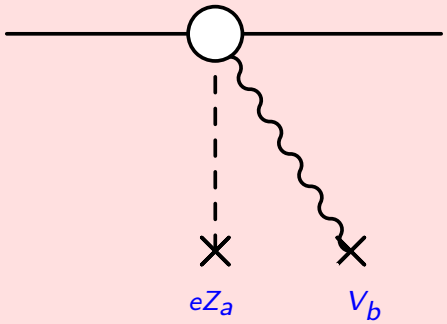


$$-e\left(Z_a\frac{\mathbf{P}_a+\mathbf{P}_a'}{2M_a}+i\,[\boldsymbol{\mu}_a\times(-\mathbf{q}]\right)$$

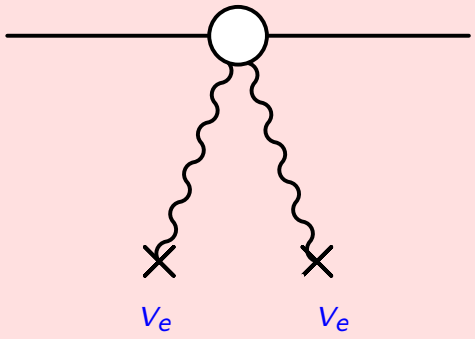
$$e^2\,\frac{\mathbf{E}^2}{8m_e^3}$$



$$e^2\,\frac{[\mathbf{A}\times\mathbf{E}]}{4m_e^2}$$



$$-e^2Z_a^2\,\frac{\mathbf{A}^2}{2M_a}$$



Spin-averaged frequency

The nonrecoil effective Hamiltonian:

$$H_1 = \frac{p^6}{16m^5} + \frac{\boldsymbol{\mathcal{E}}^2}{8m^3} - \frac{3}{64m^4}\left\{p^2, \Delta V\right\} + \frac{5}{128m^4}\left\{p^4, V\right\} - \frac{5}{64m^4}\left(p^2 V p^2\right),$$

Relativistic correction to the transverse photon

$$H_2 = \frac{1}{8m^2}\left\{p^2, \frac{p^i}{m}\left(\frac{\delta^{ij}}{r} + \frac{r^i r^j}{r^3}\right)\frac{Z_a p^j}{M_a}\right\}.$$

The double transverse photon exchange ($\frac{Z^2}{2M}\mathbf{A}^2$):

$$H_3 = \frac{Z_a^2}{8M_a}\,\frac{p^i}{m}\left(\frac{\delta^{ij}}{r} + \frac{r^i r^j}{r^3}\right)\left(\frac{\delta^{jk}}{r} + \frac{r^j r^k}{r^3}\right)\frac{p^k}{m}.$$

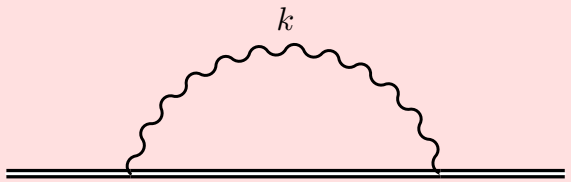
Retarded transverse photon exchange

$$H_4 = 2\left\{\frac{1}{8}\,\frac{p^i}{m}(E_0 - H_0)\left(\frac{r^i r^j}{r} - 3\delta^{ij} r\right)(E_0 - H_0)\frac{Z_a p^k}{M_a}\right\}.$$

Spin contributions at order $m(Z\alpha)^6$

Is now under consideration...

One-loop electron self-energy for a bound electron



Using QED approach for the two Coulomb center problem one may get the total contribution without expansion in terms of $(Z\alpha)$.

$$\Delta E_{se} = \frac{e^2}{i}\int \frac{d^4k}{(2\pi)^4}\,\frac{1}{k^2+i\epsilon}\left\langle \bar{\psi}\left| e^{i\mathbf{kr}}\gamma^\mu \frac{1}{H_D - E_0 + k_0}\gamma_\mu e^{-i\mathbf{kr}}\right|\psi\right\rangle$$
$$-\delta m\left\langle\bar{\psi}|\psi\right\rangle$$

Thank you for your attention!