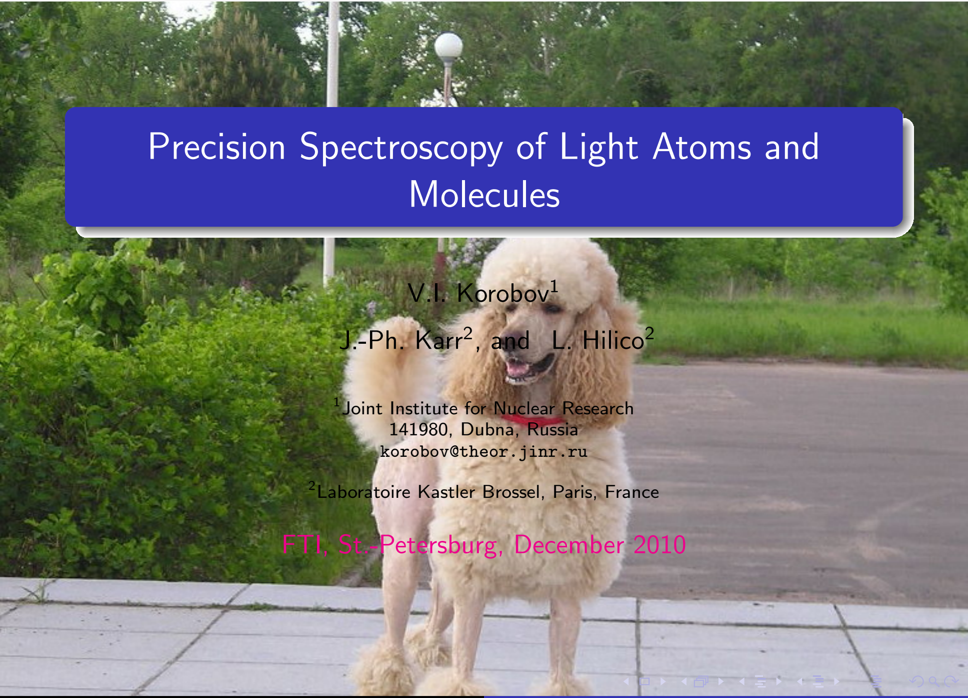


Precision Spectroscopy of Light Atoms and Molecules

V.I. Korobov[1]

J.-Ph. Karr[2], and L. Hilico[2]

[1]Joint Institute for Nuclear Research
141980, Dubna, Russia
korobov@theor.jinr.ru

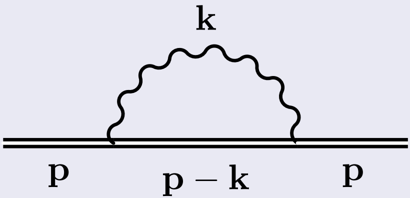
[2]Laboratoire Kastler Brossel, Paris, France

FTI, St.-Petersburg, December 2010

Hydrogen molecular ion
Contributions to the $(0,0)\to(0,1)$ transition energy.

	H_2^+	HD^+
ΔE_{nr}	65 687 511.0686	57 349 439.9717
ΔE_{α^2}	1091.041(03)	958.152(03)
ΔE_{α^3}	−276.544(02)	−242.125(02)
ΔE_{α^4}	−1.997	−1.748
ΔE_{α^5}	0.120(23)	0.105(19)
ΔE_{tot}	65 688 323.688(25)	57 350 154.355(21)

One-loop contribution in order $m\alpha^7$



General one-loop result

U. Jentschura, A. Czarnecki, and K. Pachucki, Phys. Rev. A **72**, 062102 (2005)

$$\Delta E^{(7)}_{\rm se} = \frac{\alpha}{\pi}\Biggl\{(Z\alpha)^6\mathcal{L} + \left(\frac{5}{9}+\frac{2}{3}\ln\left[\frac{1}{2}(Z\alpha)^{-2}\right]\right)\left\langle 4\pi\rho\, Q(E-H)^{-1}Q\, H_R\right\rangle$$

$$+2\left\langle H_{so}\, Q(E-H)^{-1}Q\, H_R\right\rangle + \left(\frac{779}{14400}+\frac{11}{120}\ln\left[\frac{1}{2}(Z\alpha)^{-2}\right]\right)\left\langle \boldsymbol{\nabla}^4 V\right\rangle$$

$$+\left(\frac{23}{576}+\frac{1}{24}\ln\left[\frac{1}{2}(Z\alpha)^{-2}\right]\right)\left\langle 2\mathrm{i}\sigma^{ij}p^i\boldsymbol{\nabla}^2 V p^j\right\rangle$$

$$+\left(\frac{589}{720}+\frac{2}{3}\ln\left[\frac{1}{2}(Z\alpha)^{-2}\right]\right)\left\langle \boldsymbol{\mathcal{E}}^2\right\rangle + \frac{3}{80}\left\langle 4\pi\rho\,\mathbf{p}^2\right\rangle - \frac{1}{4}\left\langle \mathbf{p}^2 H_{so}\right\rangle\Biggr\}$$

where

$$H_R = -\frac{p^4}{8} + \frac{\pi}{2}Z\alpha\delta(\mathbf{r}) + H_{so}, \qquad H_{so} = \frac{1}{4}\,\sigma^{ij}\nabla^i V p^j = Z\alpha\frac{[\mathbf{r}\times\mathbf{p}]\,\boldsymbol{\sigma}}{4r^3}\,,$$

$$\sigma^{ij} = [\sigma^i\sigma^j]/(2i) = \epsilon^{ijk}\sigma^k,$$

Defining finite operators

$$\mathcal{Q} = \lim_{r_0 \to 0} \left\{ \left\langle \frac{1}{4\pi r^3} \right\rangle_{r_0} + (\ln r_0 + \ln(Z\alpha) + \gamma_E) \langle \delta(\mathbf{r}) \rangle \right\}$$
$$= -\frac{(Z\alpha)^3}{\pi n^3} \left[\psi(n) - \psi(1) - \ln \frac{n}{2} - \frac{1}{2} + \frac{1}{2n} \right],$$

$$\mathcal{R} = \lim_{r_0 \to 0} \left\{ \left\langle \frac{1}{4\pi r^4} \right\rangle_{r_0} - \left[\frac{1}{r_0} \langle \delta(\mathbf{r}) \rangle + (\ln r_0 + \ln(Z\alpha) + \gamma_E) \langle \delta'(\mathbf{r}) \rangle \right] \right\}$$
$$= \frac{2(Z\alpha)^4}{\pi n^3} \left[\psi(n) - \psi(1) - \ln \frac{n}{2} - \frac{5}{3} + \frac{1}{2n} + \frac{1}{6n^2} \right].$$

where

$$\langle \phi_1 | \delta'(\mathbf{r}) | \phi_2 \rangle = \left\langle \phi_1 \left| \frac{\mathbf{r}}{r} \boldsymbol{\nabla} \delta(\mathbf{r}) \right| \phi_2 \right\rangle = -\langle \partial_r \phi_1 | \delta(\mathbf{r}) | \phi_2 \rangle - \langle \phi_1 | \delta(\mathbf{r}) | \partial_r \phi_2 \rangle.$$

Defining finite operators (cont.)

$$4\pi\langle V\rho\rangle = -4\pi(Z\alpha)^2\mathcal{R} - 8\pi(Z\alpha)^3\mathcal{Q} - 2E_0\left\langle V^2\right\rangle + \left\langle \mathbf{p}V^2\mathbf{p}\right\rangle$$
$$= \frac{12(Z\alpha)^6}{n^3}$$

$$4\pi\left\langle p^2\rho\right\rangle = 8\pi(Z\alpha)^2\mathcal{R} + 16\pi(Z\alpha)^3\mathcal{Q} + 4E_0\left\langle V^2\right\rangle - 2\left\langle \mathbf{p}V^2\mathbf{p}\right\rangle + 2E_0\langle 4\pi\rho\rangle$$
$$= \frac{8(Z\alpha)^6}{n^3}\left[-3 - \frac{1}{2n^2}\right]$$

$$\left\langle \left[\boldsymbol{\nabla}^4 V\right]\right\rangle = -16\pi(Z\alpha)^2\mathcal{R} - 32\pi(Z\alpha)^3\mathcal{Q} - 8E_0\left\langle V^2\right\rangle + 4\left\langle \mathbf{p}V^2\mathbf{p}\right\rangle$$
$$+2\langle \mathbf{p}(4\pi\rho)\mathbf{p}\rangle - 4E_0\langle 4\pi\rho\rangle$$
$$= \frac{8(Z\alpha)^6}{n^3}\left[7 + \frac{1}{n^2}\right]$$

The second order contribution

$$\left\langle 4\pi\rho\, Q(E-H)^{-1}Q\, \left(-\frac{p^4}{8}+\frac{\pi}{2}\,\rho\right)\right\rangle = \left\langle H'^{(1)}\, Q(E-H)^{-1}Q\, H'^{(2)}\right\rangle$$
$$+\frac{1}{4}\left[4\pi(Z\alpha)^2\mathcal{R} + 16\pi(Z\alpha)^3\mathcal{Q} + 8E_0\left\langle V^2\right\rangle - 4E_0^2\left\langle V\right\rangle\right.$$
$$\left. + \left\langle H^{(1)}\right\rangle\langle V\rangle - 8\left\langle H^{(2)}\right\rangle\langle V\rangle\right]$$

$$= \frac{2(Z\alpha)^6}{n^3}\left[-\ln(2) - \psi(n) + \psi(1) + \ln n + \frac{1}{2} + \frac{1}{n} - \frac{5}{2n^2}\right].$$

Here we use the transformation

$$H'^{(1)} = -(E_0 - H_0)U_1 - U_1(E_0 - H_0) + H^{(1)} \qquad U_1 = 2V,$$
$$H'^{(2)} = -(E_0 - H_0)U_2 - U_2(E_0 - H_0) + H^{(2)}, \qquad U_2 = -\frac{1}{4}V.$$

Comparison with the hydrogen $1S$ state

The finite result from the redefined Jentschura, Czarnecki, Pachucki expression:

$$\Delta E_{\rm se}^{(7)}(1S) = \frac{\alpha(Z\alpha)^6}{\pi}\biggl\{\mathcal{L}(1S) - 2\left(\frac{5}{9}+\frac{2}{3}\ln\left[\frac{1}{2}(Z\alpha)^{-2}\right]\right)\Bigl[\ln(2)+1\Bigr]$$

$$+64\left(\frac{779}{14400}+\frac{11}{120}\ln\left[\frac{1}{2}(Z\alpha)^{-2}\right]\right)$$

$$+8\left(\frac{589}{720}+\frac{2}{3}\ln\left[\frac{1}{2}(Z\alpha)^{-2}\right]\right)\Bigl[\ln(2)-1\Bigr] - 28\frac{3}{80} + C\biggr\}$$

That should be compared with

$$\Delta E_{\rm se}^{(7)}(1S) = \frac{\alpha(Z\alpha)^6}{\pi}\biggl\{-\ln^2\left[(Z\alpha)^{-2}\right] + \left[\frac{28}{3}\ln 2 - \frac{21}{20} - \frac{2}{15}\right]\ln\left[(Z\alpha)^{-2}\right]$$

$$-30.92414946(1)\biggr\}$$

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$$-30.92414946(1)\Biggr\}$$

from that one gets

$$C = -\ln^2\left[(Z\alpha)^{-2}\right] + \left[\frac{16}{3}\ln 2 - \frac{23}{60}\right]\ln\left[(Z\alpha)^{-2}\right] - 0.81971202(1)$$

Low energy contribution
Relativistic Bethe Log

Definitions

U. Jentschura, A. Czarnecki, and K. Pachucki, Phys. Rev. A **72**, 062102 (2005)

$$E_{L1} = \frac{2\alpha^5}{3\pi}\int_0^\Lambda k\,dk\;\delta_{H_B}\left\langle \mathbf{p}\left(\frac{1}{E_0-H-k}\right)\mathbf{p}\right\rangle = \frac{2\alpha^5}{3\pi}\int_0^\Lambda k\,dk\;P_{rd}^{(1)}(k)$$

$$E_{L2} = \frac{2\alpha^5}{3\pi}\int_0^\Lambda k\,dk\;P_{nq}(k)$$

$$E_{L3} = \frac{4\alpha^5}{3\pi}\int_0^\Lambda k\,dk\left\langle \delta\mathbf{j}\left(\frac{1}{E_0-H-k}\right)\mathbf{p}\right\rangle = \frac{2\alpha^5}{3\pi}\int_0^\Lambda k\,dk\;P_{rd}^{(2)}(k)$$

where

$$P_{rd}^{(1)}(k) = 2\left\langle H_B Q (E_0-H)^{-1} Q\mathbf{p}\,(E_0-H-k)^{-1}\,\mathbf{p}\right\rangle + \left\langle \mathbf{p}\,(E_0-H-k)^{-1}\Big(H_B+\langle H_B\rangle\Big)(E_0-H-k)^{-1}\,\mathbf{p}\right\rangle$$

$$P_{nq}(k) = \frac{3}{8\pi}\int_S dS_{\mathbf{n}}\left(\delta^{ij}-n^i n^j\right)\Big\{\left\langle p^i(\mathbf{n}\cdot\mathbf{r})\,(E_0-H-k)^{-1}\,(\mathbf{n}\cdot\mathbf{r})p^i\right\rangle - \left\langle p^i(\mathbf{n}\cdot\mathbf{r})^2\,(E_0-H-k)^{-1}\,p^i\right\rangle\Big\}$$

$$P_{rd}^{(2)}(k) = \left\langle\left(-p^2p^i-\frac{1}{2}\sigma^{ij}\nabla^j V\right)(E_0-H-k)^{-1}\,p^i\right\rangle$$

Asymptotics $k \to \infty$
Wavefunction ψ_1

The first order nonrelativistic perturbation wave function is determined by

$$(E_0 - H - k)\psi_1 = \boldsymbol{\nabla}\psi_0,$$

It can be approximately expressed by ($\mu = \sqrt{2k}$)

$$\psi_1(\mathbf{r}) \approx -\frac{1}{k}\boldsymbol{\nabla}\psi_0(r) - \frac{\mathbf{r}}{r}\frac{Z}{k^2 r^2}\left[1 - e^{-\mu r}(1 + \mu r)\right]\psi_0(r),$$

which has a proper behaviour at $r \to 0$.

For the nonrelativistic dipole term

$$P_{nd}(k) = \frac{1}{k}\left\langle \boldsymbol{\nabla}^2 \right\rangle + \frac{Z}{2k^2}\,4\pi\left\langle \delta(\mathbf{r})\right\rangle - \frac{Z^2(\sqrt{2k} - Z\ln k)}{k^3} 4\pi\left\langle \delta(\mathbf{r})\right\rangle + \dots$$

The other terms may be expressed

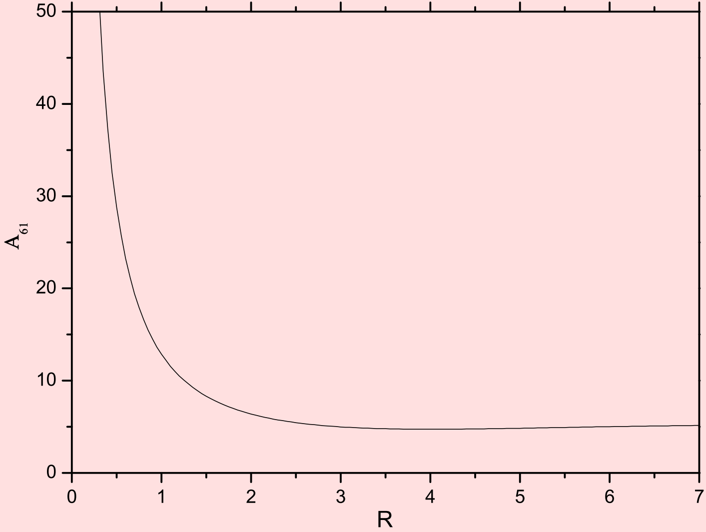
$$P_{nq}(k) = -\frac{k}{2}P_{nd}(k) - \frac{1}{5k}\left\langle \nabla^4 \right\rangle - \frac{Z}{4k}\,4\pi\left\langle \delta(\mathbf{r})\right\rangle + \frac{3Z^2(\sqrt{2k} - Z\ln k)}{2k^2}\,4\pi\left\langle \delta(\mathbf{r})\right\rangle + \dots$$

$$P_{rd}^{(1)}(k) = \frac{2}{k}\left\langle (H_R - \langle H_R\rangle)\,(E_0 - H)^{-1}\boldsymbol{\nabla}^2 \right\rangle + \frac{Z^2(\sqrt{2k} + Z\ln k)}{4k^2}\,4\pi\left\langle \delta(\mathbf{r})\right\rangle + \dots$$

$$P_{rd}^{(2)}(k) = \frac{\left\langle p^4 \right\rangle}{k} + \frac{Z^2(-2\sqrt{2k} + Z\ln k)}{k^2}\,4\pi\left\langle \delta(\mathbf{r})\right\rangle + \dots$$

$$\boxed{A_{62} = -1}$$

Coefficient A_{61}

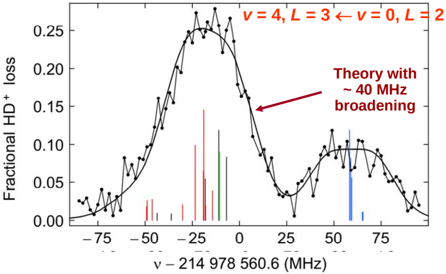


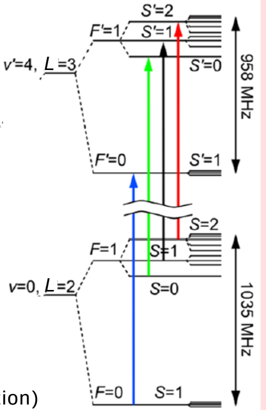
Experiment

High-resolution spectrum of overtone transition

Koelemeij, Roth, Wicht, Ernsting, Schiller, PRL 98, 173002 (2007)

- 1.39 μm diode laser (300 kHz linewidth) locked to a Ti:Sa frequency comb, stabilized to a H-maser & GPS.
  Wicht et al, Appl. Phys. B 78, 137 (2004); Strauss et al, Appl. Phys. B 88, 21 (2007)





- Transition frequency (without hyperfine contribution)

  $\nu = 214\,978\,560.6 \pm 0.5$ MHz

- Theoretical value (*V. Korobov PRA 77, 022509 (2008), using CODATA02*)

  $\nu = 214\,978\,560.88 \pm 0.07$ MHz

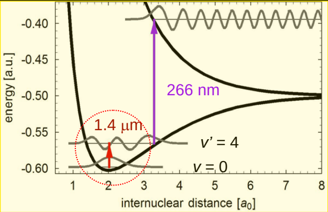
Hydrogen molecular ion
Amsterdam Experiment

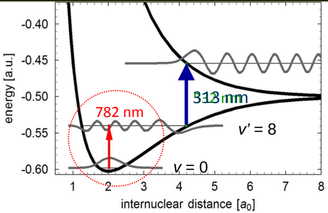
HD^+ spectroscopy at VU Amsterdam

- First demonstrated at Düsseldorf *:
  - 170 µW at 1.4 µm
  - several mW at 266 nm
  - beam waists ~150 µm
  - observe REMPD loss of HD^+

- LaserLaB approach:
  - Overtone v=0 – v'=8 @782 nm
  - Einstein B-coefficient 1000× smaller
  - Need ~200 mW in 150 µm
  - REMPD by (780 + 532) nm

    OR by (780 + 313) nm

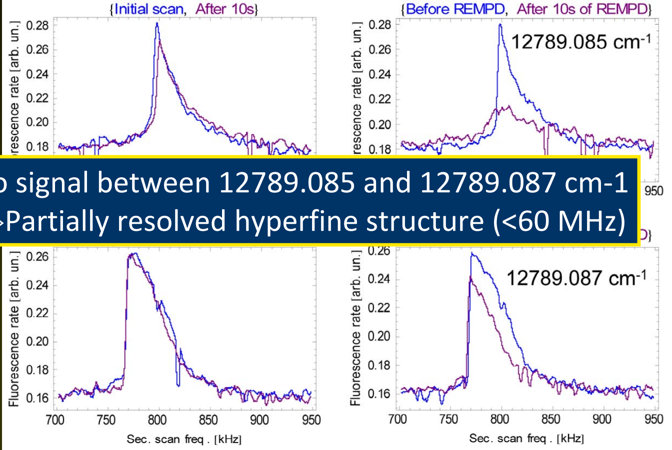




* B. Roth, JK, H. Daerr, S. Schiller *Phys. Rev. A* **74**, 040501(R) (2006)

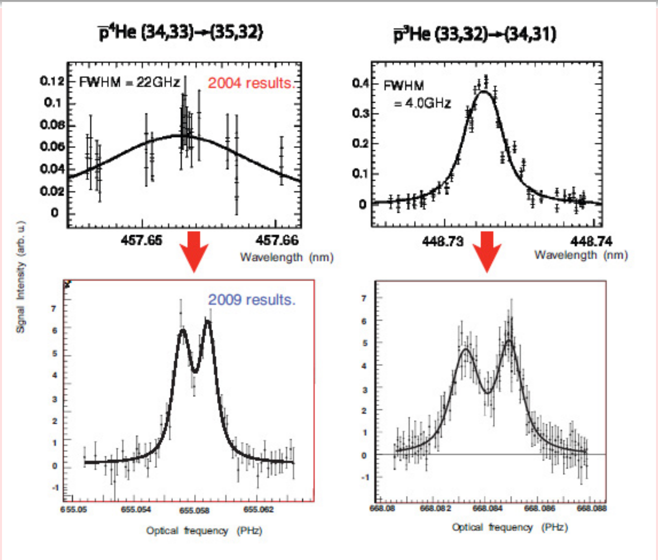
JK, B. Roth, A. Wicht, I. Ernsting, S. Schiller, *Phys. Rev. Lett.* **98**, 173002 (2007)

First observation of $v=0 \rightarrow v'=8$ in HD^+



No signal between 12789.085 and 12789.087 cm-1
⇒Partially resolved hyperfine structure (<60 MHz)

Antiprotonic Helium
Experiment: 2009 vs 2004



Thank you for your attention!