Fine structure of helium-like atoms and the fine-structure constant

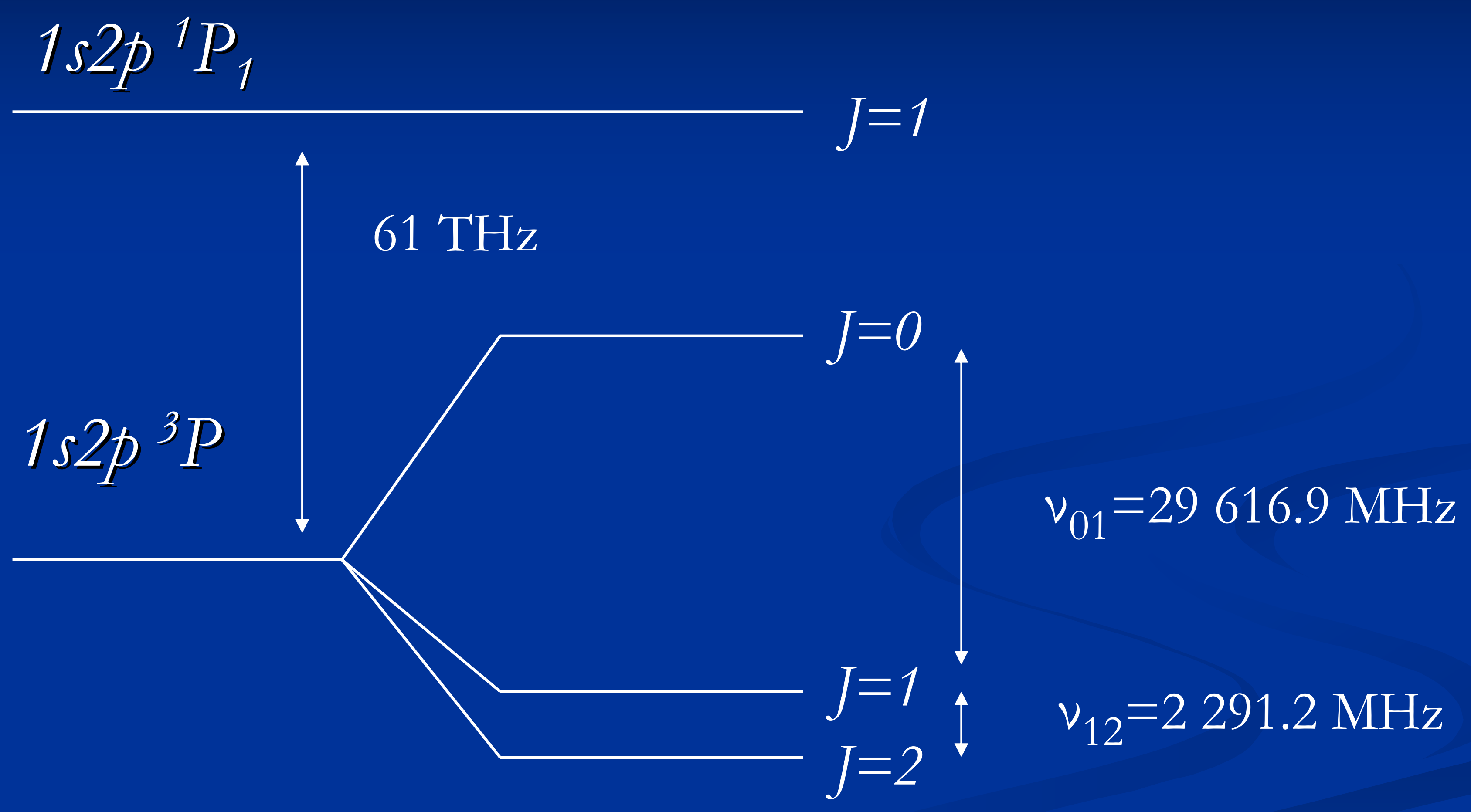
K. Pachucki
Institute of Theoretical Physics, University of Warsaw

V. A. Yerokhin
St. Petersburg State Polytechnical University

Supported by NIST Precision Measurement Grant

December 9, St. Petersburg, FFK 2010

Structure of the *2P* states of helium



$\nu_{02}=\nu_{01}+\nu_{12}=31\ 908.1$ MHz

Spectroscopic determination of the fine-structure constant

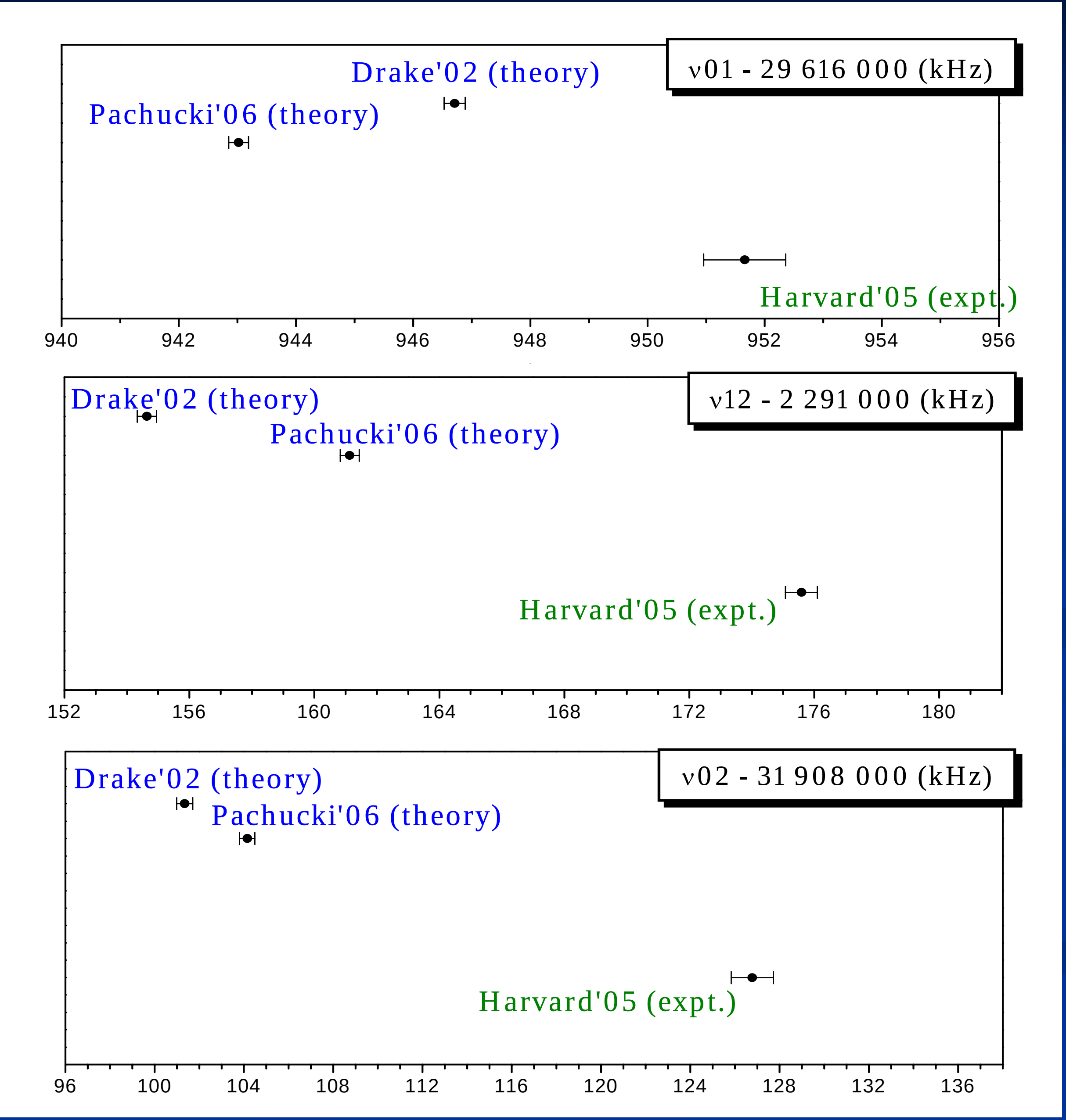
- Early determinations of α were made from the hydrogen fine structure (1954, 10 ppm) and were limited by the short lifetime of the *2p* state.

- Schwartz 1964: the lifetime of the 2^3P state of helium is two orders of magnitude longer. Theoretical description is difficult but possible.

- Lewis and Serafino 1978: calculation of the helium fine structure up to order $m\alpha^6$. Determination of α up to 0.9 ppm.

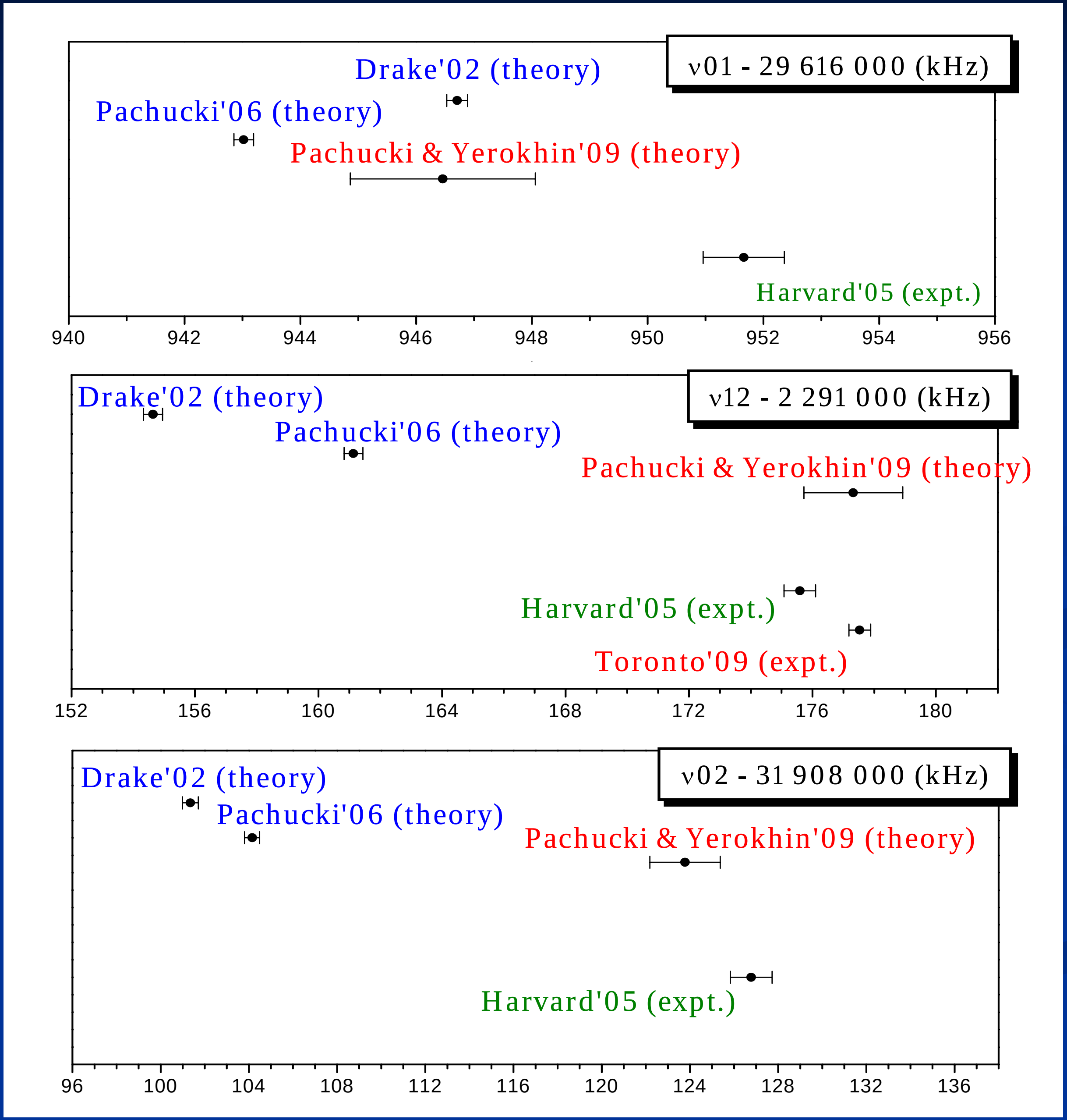
- Present experimental precision is sufficient to determine α with a 5 ppb accuracy, which is comparable with the second-best determination of α (4.6 ppb) from the atomic recoil effect.

Theory and experiment: status 2006



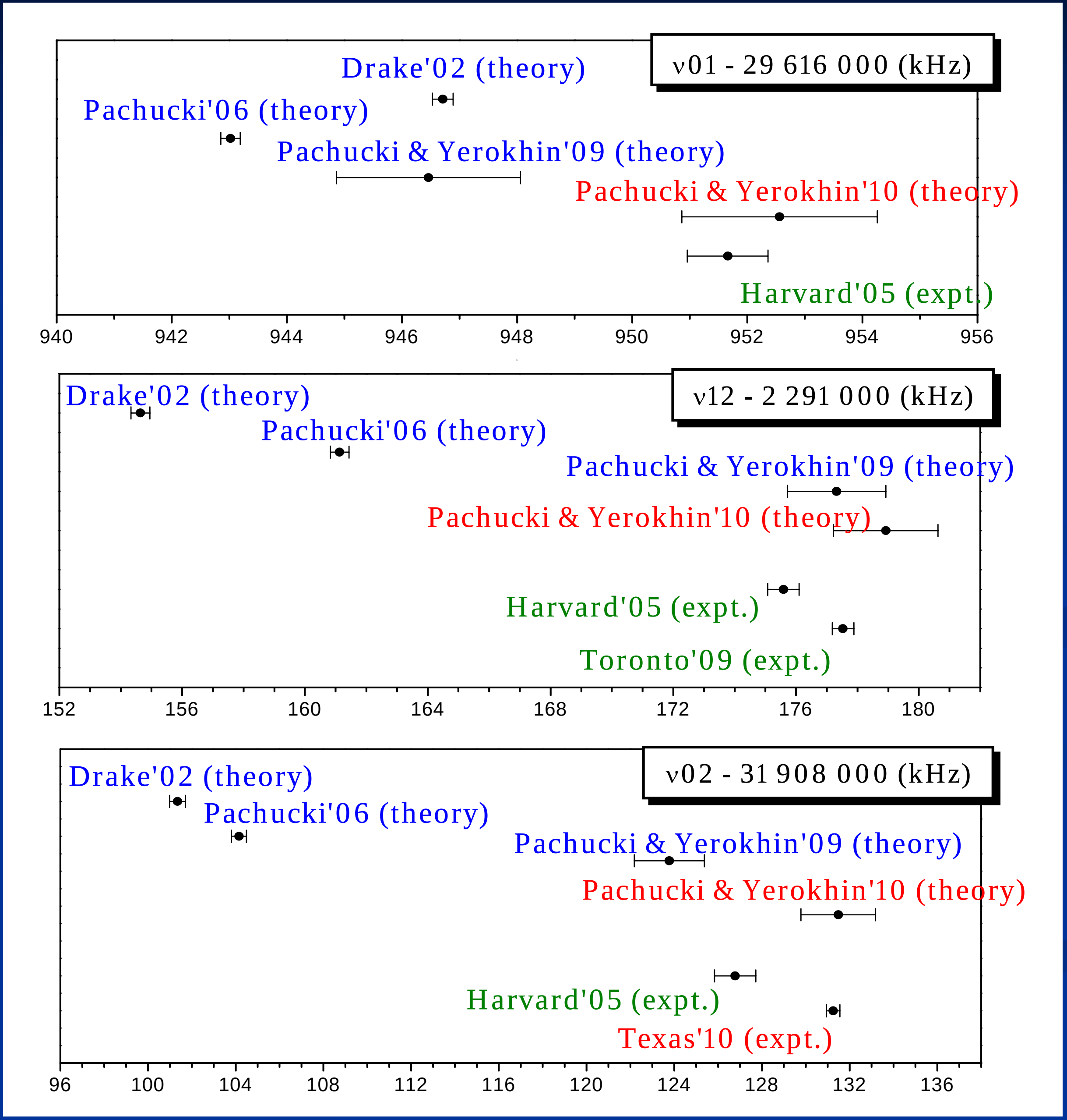
*All theories are scaled to the present value of α

Theory and experiment: status 2009



*All theories are scaled to the present value of α

Theory and experiment: status 2010



K. Pachucki and V.A. Yerokhin, Phys. Rev. Lett. **104**, 070403 (2010)

*All theories are scaled to the present value of α

Theory of the fine structure of light atoms

Expansion of the energy in powers of the fine-structure constant α

$$E_{\mathrm{fs}} = m \left[\alpha^4 \mathcal{E}^{(4)} + \alpha^5 \mathcal{E}^{(5)} + \alpha^6 \mathcal{E}^{(6)} + \alpha^7 \mathcal{E}^{(7)} + \ldots \right],$$

and the electron-to-nucleus mass ratio *m/M*

$$\mathcal{E}^{(n)} = \mathcal{E}^{(n)}_{\infty} + (m/M)\, \mathcal{E}^{(n)}_{M} + \ldots$$

- Expansion is valid for systems with small nuclear charges *Z*

- Expansion coefficients are expressed in terms of matrix elements of some effective Hamiltonians with the nonrelativistic wave function of the reference state

Fine structure: main contribution

Main contribution is given by the matrix element of the Breit Hamiltonian with the electron anomalous magnetic moment included. It includes all $m\alpha^4$ and $m\alpha^5$ effects. In the non-recoil limit, the effective Hamiltonian is

$$
\begin{aligned}
H_{\rm fs} \;=\; & \frac{\alpha}{4\,m^2}\left(\frac{\vec\sigma_1\cdot\vec\sigma_2}{r^3} - 3\,\frac{\vec\sigma_1\cdot\vec r\,\vec\sigma_2\cdot\vec r}{r^5}\right)(1+a_e)^2 \\
& + \frac{Z\alpha}{4m^2}\left[\frac{1}{r_1^3}\,\vec r_1\times\vec p_1\cdot\vec\sigma_1 + \frac{1}{r_2^3}\,\vec r_2\times\vec p_2\cdot\vec\sigma_2\right](1+2a_e) \\
& + \frac{\alpha}{4\,m^2\,r^3}\Big[\left[(1+2\,a_e)\,\vec\sigma_2 + 2\,(1+a_e)\,\vec\sigma_1\right]\cdot\vec r\times\vec p_2 \\
& - \left[(1+2\,a_e)\,\vec\sigma_1 + 2\,(1+a_e)\,\vec\sigma_2\right]\cdot\vec r\times\vec p_1\Big],
\end{aligned}
$$

where $\vec r = \vec r_1 - \vec r_2$ and a_e is the electron anomalous magnetic moment,

$$
a_e \;=\; \frac{\alpha}{2\pi} - 0.328\,478\,965\left(\frac{\alpha}{\pi}\right)^2 + 1.181\,241\,456\left(\frac{\alpha}{\pi}\right)^3 + \ldots\,.
$$

Higher-order corrections

Contribution of order $m\alpha^6$:

$$\mathcal{E}^{(6)} = \left\langle H^{(6)} \right\rangle + \left\langle H^{(4)} \frac{1}{(E_0 - H_0)'} H^{(4)} \right\rangle$$

Contribution of order $m\alpha^7$

$$\mathcal{E}^{(7)} = \left\langle H^{(7)} \right\rangle + 2 \left\langle H^{(5)} \frac{1}{(E_0 - H_0)'} H^{(4)} \right\rangle + \mathcal{E}_L \,,$$

where $\mathcal{E}_L$ is the relativistic correction to the Bethe logarithm.

Nonrelativistic energy and wave function

Korobov 2000, 2002

- Wave function

$$\vec{\phi}(\vec{r}_1, \vec{r}_2) = \sum_i c_i \left[\vec{r}_1 \, \exp(-\alpha_i \, r_1 - \beta_i \, r_2 - \gamma_i \, r_{12}) - (1 \leftrightarrow 2) \right].$$

- Variational approach: minimize energy with respect to α_i, β_i, γ_i, and c_i.
- Master integral:

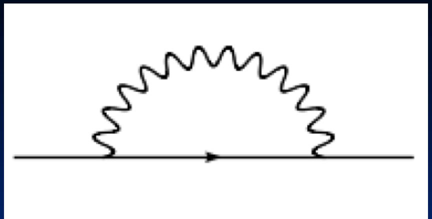
$$\frac{1}{16\pi^2} \int d^3 r_1 \, d^3 r_2 \, \frac{e^{-\alpha \, r_1 - \beta \, r_2 - \gamma \, r_{12}}}{r_1 \, r_2 \, r_{12}} = \frac{1}{(\alpha + \beta)(\beta + \gamma)(\gamma + \alpha)}.$$

- Parameters α_i, β_i, and γ_i are chosen quasirandomly from the intervals $\alpha_i \in [A_1, A_2]$, $\beta_i \in [B_1, B_2]$, $\gamma_i \in [C_1, C_2]$. $A_{1,2}$, $B_{1,2}$, and $C_{1,2}$ are determined by a variational optimization.
- Norelativistic energy:

$$E_0(2^3P) = -2.133\,164\,190\,779\,283\,205\,146\,96^{+0}_{-10} \quad \text{(23 digits)}$$

- Octuple arithmetics (appr. 72 digits) is required for calculations.

Bethe logarithm for helium



Two main representations:

I) The integral representation (Schwartz 1961, Korobov and Korobov 1999):

$$\ln k_0 \overset{K\to\infty}{=} \frac{1}{\mathcal{D}} \int_0^K dk\, k \left\langle \vec{\nabla} \frac{1}{E_0 - H_0 - k} \vec{\nabla} \right\rangle - A\,K - B\,\ln K\,,$$

where $\mathcal{D} = 2\pi Z \langle \delta^3(r_1) + \delta^3(r_2) \rangle$, $\vec{\nabla} \equiv \vec{\nabla}_1 + \vec{\nabla}_2$, and A and B are the constants of a large-k expansion of the integrand.

II) The sum over the spectrum (Drake and Goldman 1999 , Korobov 2004):

$$\ln k_0 = \frac{1}{\mathcal{D}} \sum_n |\langle 0|\,\vec{\nabla}\,|n\rangle|^2 (E_n - E_0) \ln |E_n - E_0|\,.$$

Bethe logarithm for the 2^3P state of helium:

$$\begin{aligned} \ln(k_0/Z^2) \quad = \quad & 2.983\,691\,003\,3\,(2) \quad \text{our result} \\ & 2.983\,690\,995\,(1) \quad \text{Korobov 2004} \\ & 2.983\,690\,84\,(2) \quad \text{Drake and Goldman 1999} \end{aligned}$$

Relativistic correction to the Bethe logarithm

The nonrelativistic Hamiltonian H_0, energy E_0, wave function ψ, and current $\vec{\nabla}$ are modified by relativistic corrections:

$$H_0 \to H_0 + H^{(4)}\,, \quad E_0 \to E_0 + E^{(4)}\,, \quad \psi \to \psi + \delta\psi\,, \quad \vec{\nabla} \to \vec{\nabla} + \delta\vec{j}\,.$$

The result is

$$\mathcal{E}_L^{(7)} \stackrel{K\to\infty}{=} -\frac{2}{3\pi}\int_0^K dk\,k\left\{2\left\langle\delta\psi\middle|\vec{\nabla}\frac{1}{H_0+k-E_0}\vec{\nabla}\middle|\psi\right\rangle\right.$$
$$+\left\langle\vec{\nabla}\frac{1}{H_0+k-E_0}\left[\delta E^{(4)}-H^{(4)}\right]\frac{1}{H_0+k-E_0}\vec{\nabla}\right\rangle$$
$$\left.+2\left\langle\delta\vec{j}\frac{1}{H_0+k-E_0}\vec{\nabla}\right\rangle\right\} - A\,K - B\,\ln K\,,$$

where $\delta\psi$ and $\delta E^{(4)}$ are first-order perturbations of the wave function and the reference-state energy by $H^{(4)}$.

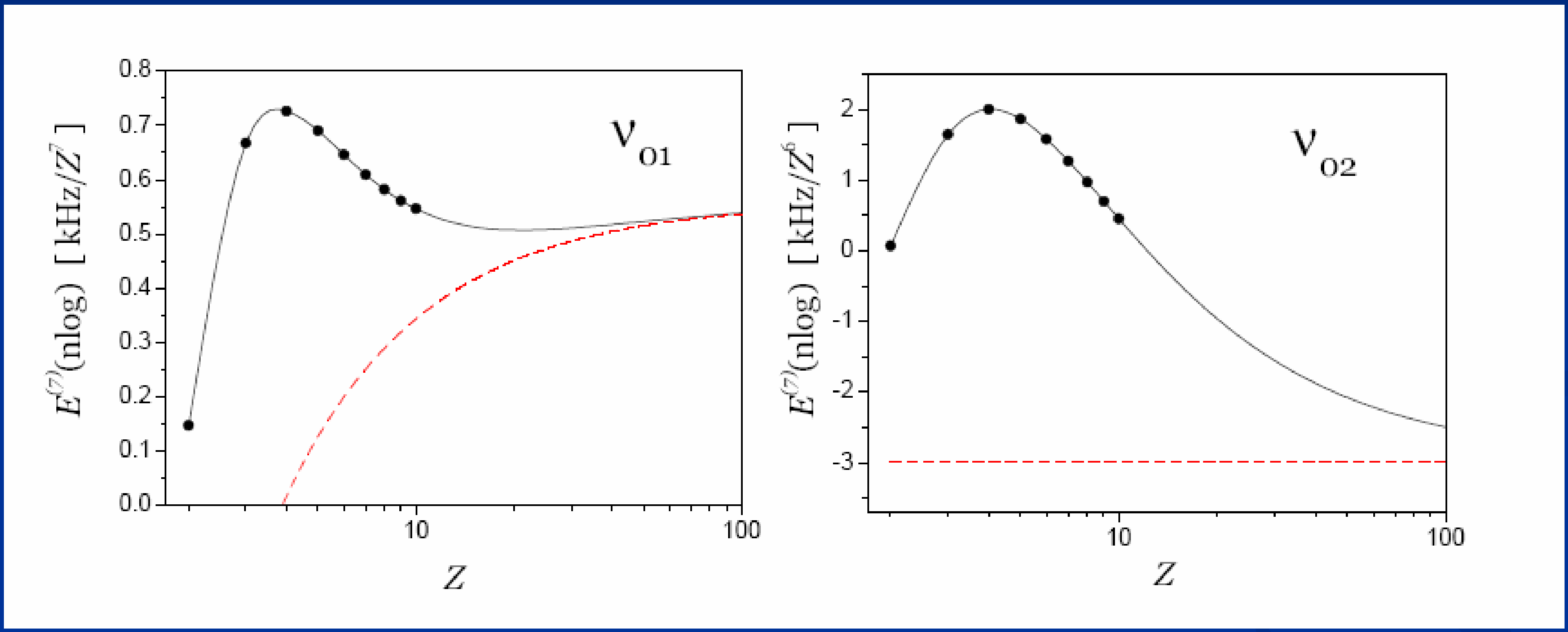
Helium fine structure: results

Term	ν_{01}	ν_{12}	
$m\alpha^4(+m/M)$	29 563 765.45	2 320 241.43	
	29 563 765.23[a]	2 320 241.42[a]	Drake'02
$m\alpha^5(+m/M)$	54 704.04	−22 545.00	
	54 704.04	−22 545.01	Drake'02
$m\alpha^6$	−1 607.52(2)	−6 506.43	
	−1 607.61(4)	−6 506.45(7)	Drake'02
$m\alpha^6 m/M$	−9.96	9.15	
	−10.37(5)	9.80(11)	Drake'02
$m\alpha^7 \log(Z\alpha)$	81.43	−5.87	
	81.42[b]	−5.87[b]	Drake'02
$m\alpha^7$, nlog	18.86	−14.38	
$m\alpha^8$	±1.7	±1.7	
Total theory	29 616 952.29 ± 1.7	2 291 178.91 ± 1.7	
Experiment	29 616 951.66(70)[c]	2 291 177.53(35)[f]	
	29 616 952.7(10)[d]	2 291 175.59(51)[c]	
	29 616 950.9(9)[e]	2 291 175.9(10)[g]	

[c] Zelevinsky'05. [d] Giusfredi'05. [e] George'01. [f] Borbely'09. [g] Castillega'00.

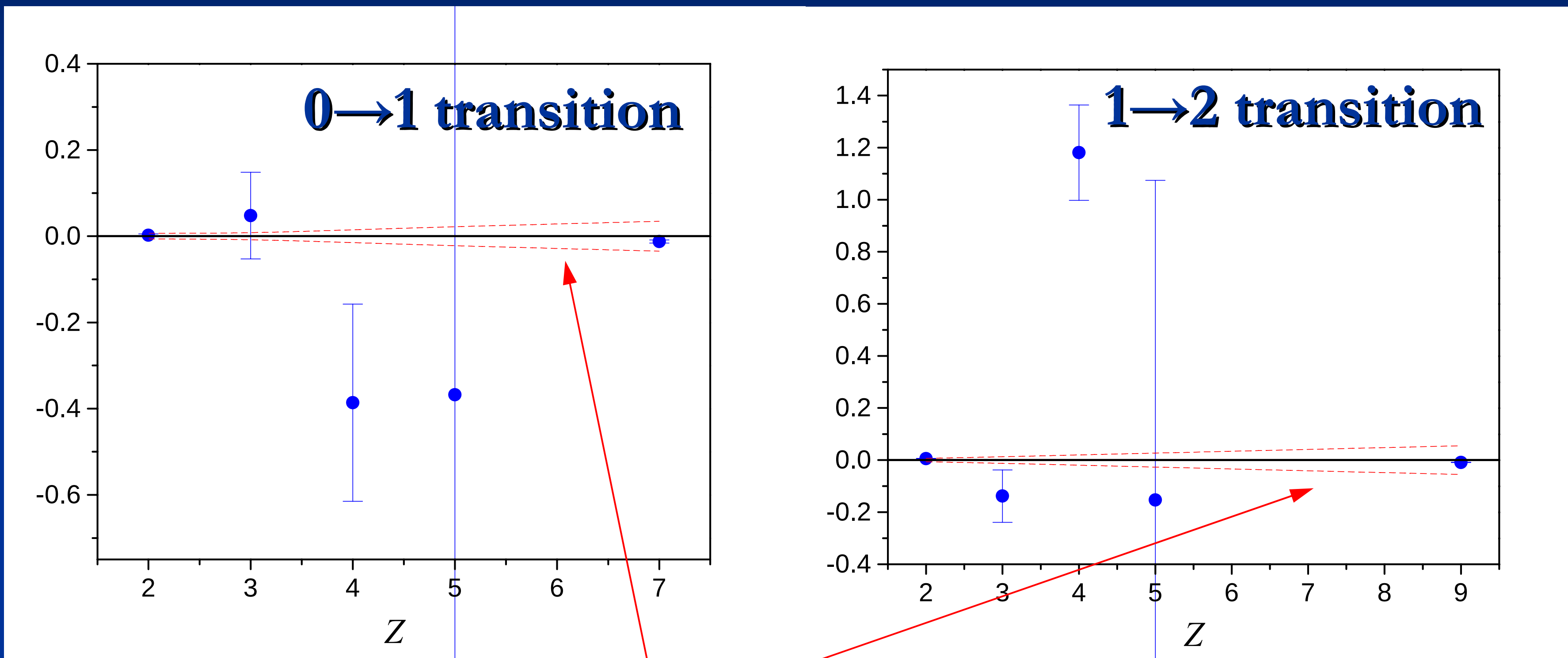
Tests: checking the hydrogenic limit

nonlogarithmic mα^7 correction, in kHz/Z^7 and kHz/Z^6



Tests: comparison with experiment for different nuclear charges

Differences theory-experiment, in kHz/Z^8



Higher-order effects (== theoretical uncertainty)

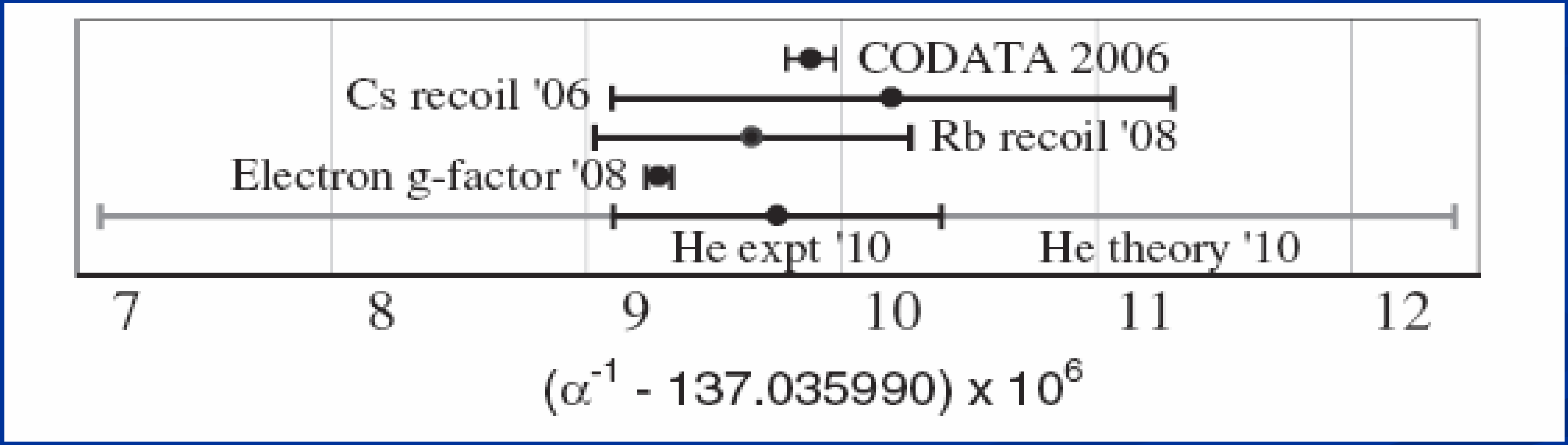
Experiments:

Z=3 Riis et al. 1994
Z=4 Scholl et al. 1993
Z=5 Dinneen et al. 1991
Z=7 Thompson et al. 1998
Z=9 Myers et al. 1999

Determination of the fine structure constant

Combining our theoretical prediction and the experimental result by Smiciklas and Shiner [Phys. Rev. Lett. 105, 123001 (2010)] for the $0 \to 2$ interval in helium, the fine-structure constant is determined with an accuracy of 29 ppb:

$$\alpha^{-1} = 137.035\,999\,55\,(64)_{exp}(4)_{num}(390)_{h.o.}$$



From Smiciklas and Shiner'10

Conclusions

- Theory and experiment agree for the fine-structure intervals in helium as well as in He-like ions.
- One of the most accurate tests of QED in light systems.
- Comparison of theoretical and experimental results determines the fine structure constant with an accuracy of 29 ppb.
- Main uncertainty of determination comes from the higher-order effects.
- Potential for further improvement (experimental determination of higher-order contribution).