International Conference on Precision Physics of Simple Atomic Systems

University of Windsor, July 21-26, 2008

Fundamental constants and tests of theory in Rydberg states of hydrogen-like ions

Ulrich Jentschura,[1,2] Peter Mohr,[1] Joseph Tan,[1] Benedikt Wundt[2]

[1]National Institute of Standards and Technology, Gaithersburg, MD, USA
[2]Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Outline

- Introduction
- Rydberg constant and the proton radius
- Rydberg ion states
- QED in Rydberg states
- Uncertainties in the theory
- Conclusion

Introduction

Comparison of precision frequency measurements to quantum electrodynamics (QED) predictions for Rydberg states of hydrogen-like ions can yield information on values of fundamental constants and test theory.

For suitable transitions, the uncertainty in the theory of the energy levels is sufficiently small that such a comparison can yield an improved value of the Rydberg constant.

U. D. Jentschura, P. J. Mohr, J. N. Tan, B. J. Wundt,
Phys. Rev. Lett. **100**, 160404 (2008).

CODATA 2006 Least-squares adjustment of the fundamental constants - references

"CODATA recommended values of the fundamental physical constants: 2006"

P. J. Mohr, B. N. Taylor, and D. B. Newell

Reviews of Modern Physics, **80**, 633 (2008)

Journal of Physical and Chemical Reference Data **37**, 1187 (2008)

Values of the constants: physics.nist.gov/constants

Bibliography on constants: physics.nist.gov/constantsbib

Hydrogen and deuterium frequencies: physics.nist.gov/hdel

Fundamental Constants from the Least-Squares Adjustment

- Hydrogen and deuterium spectra related constants
  - Rydberg constant - R_∞ [6.6 x 10^{-12}]
  - Proton rms charge radius - R_p [7.8 x 10^{-3}]
  - Deuteron rms charge radius - R_d [1.3 x 10^{-3}]
- Constants determined mainly by other data
  - fine-structure constant
  - electron-proton mass ratio
  - electron-deuteron mass ratio
- Relevant input data
  - 23 transition frequencies in H and D ≥ [1.4 x 10^{-14}]
  - R_p and R_d electron scattering data

Rydberg constant from the LSA

Experiment:

$$\nu_{\rm H}(1{\rm S}_{1/2} - 2{\rm S}_{1/2}) = 2\,466\,061\,413\,187.074(34)\ {\rm kHz} \qquad [1.4\times 10^{-14}]$$

MPQ (2006)

Theory:

$$\nu_{\rm H} = \frac{3}{4} R_\infty c \left[1 - \frac{m_{\rm e}}{m_{\rm p}} + \frac{11}{48}\alpha^2 - \frac{28}{9}\frac{\alpha^3}{\pi}\ln\alpha^{-2} - \frac{14}{9}\left(\frac{\alpha R_{\rm p}}{\lambda\!\!\!^{-}_{\rm C}}\right)^2 + \cdots \right]$$

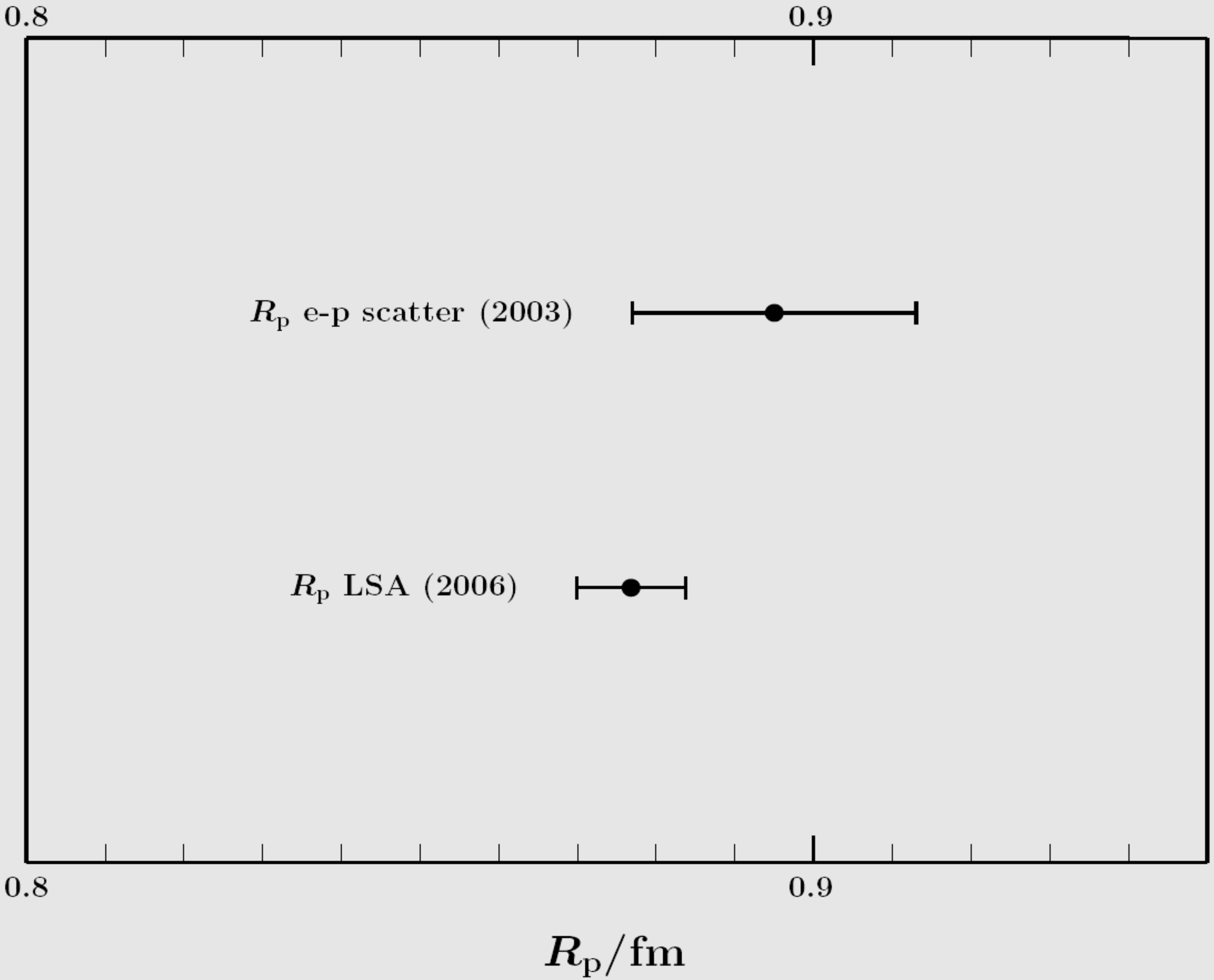
QED proton radius

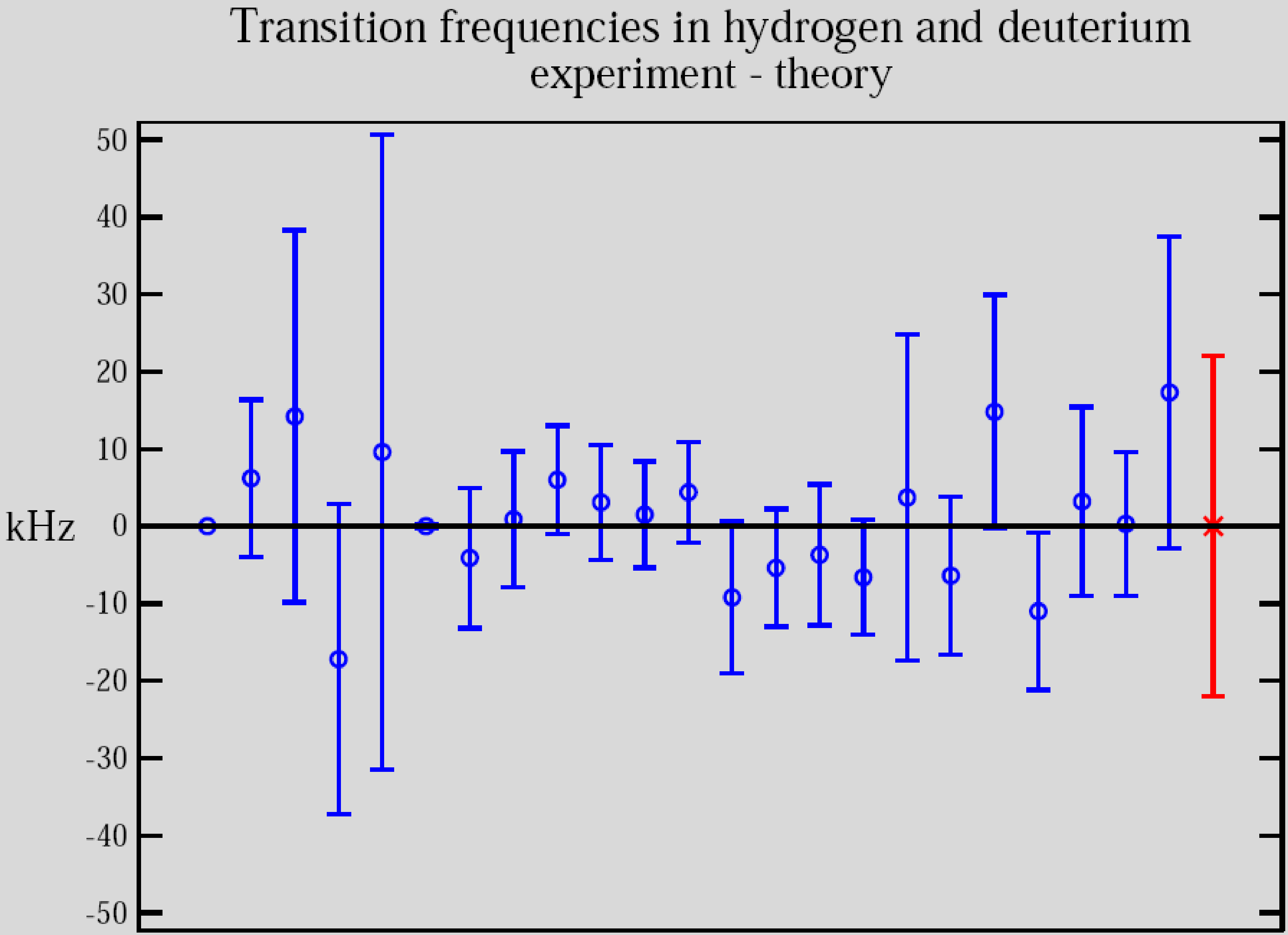
Theory reviews:

M. I. Eides, H. Grotch, V.Shelyuto, Phys. Reports **342,** 63 (2001).

J. R. Sapirstein and D. R. Yennie, in QED, ed. by T. Kinoshita (1990).

Proton charge radius from 2006 least squares adjustment





Transition frequencies in hydrogen and deuterium
experiment - theory
kHz
50
40
30
20
10
0
-10
-20
-30
-40
-50

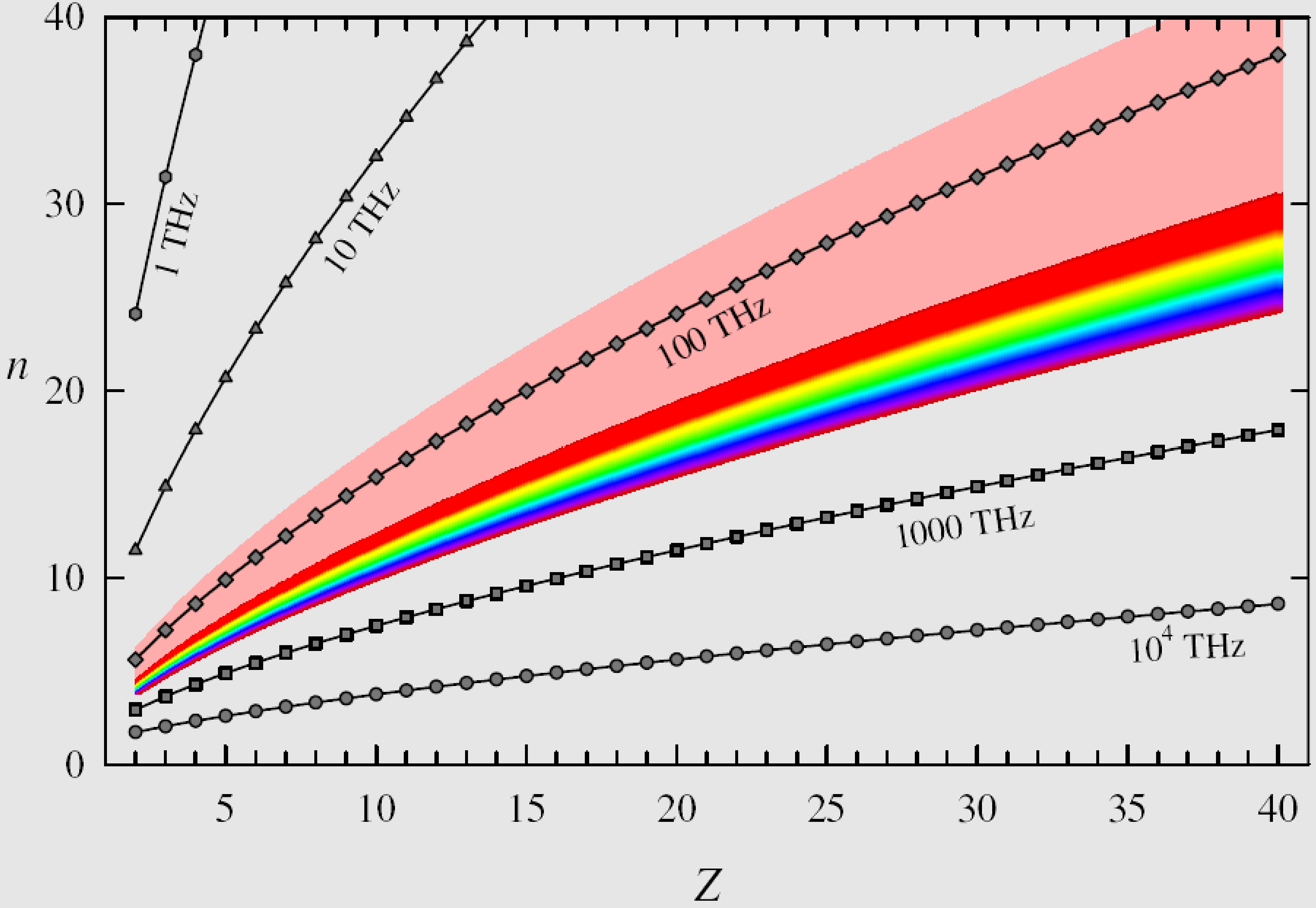
Rydberg states of hydrogen-like ions

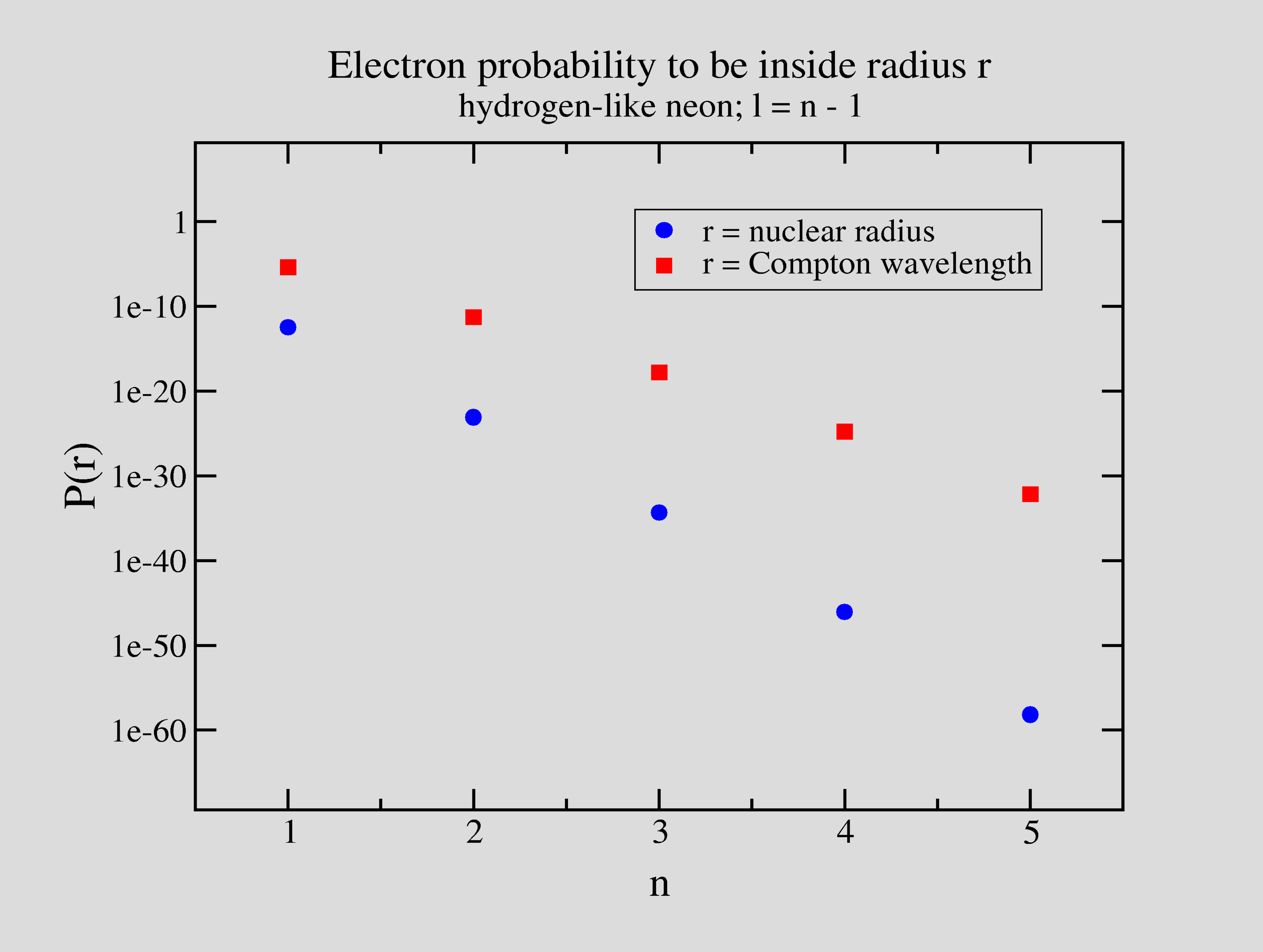
Possible means to measure the Rydberg constant

- Frequencies accessible with frequency comb lasers
- Small overlap with nucleus - no finite size correction
- Higher-order QED corrections are small

$$P(r) = \int_{|\boldsymbol{x}| \leq r} \mathrm{d}\boldsymbol{x} \, |\psi(\boldsymbol{x})|^2 \approx \frac{1}{(2n+1)!} \left(\frac{2Zr}{na_0} \right)^{2n+1}$$

Transition frequencies in hydrogen-like ions





Electron probability to be inside radius r
hydrogen-like neon; l = n - 1
r = nuclear radius
r = Compton wavelength
1
1e-10
1e-20
1e-30
1e-40
1e-50
1e-60
P(r)
1
2
3
4
5
n

Theory of Rydberg states for l ≥ 2

$$
\begin{aligned}
E_n &= E_{\mathrm{DM}} + E_{\mathrm{RR}} + E_{\mathrm{QED}} \\
E_{\mathrm{DM}} &= 2hcR_\infty \left[\mu_{\mathrm{r}} D - \frac{r_{\mathrm{N}} \mu_{\mathrm{r}}^3 \alpha^2}{2} D^2 + \frac{r_{\mathrm{N}}^2 \mu_{\mathrm{r}}^3 Z^4 \alpha^2}{2n^3 \kappa (2l+1)} \right] \\
E_{\mathrm{RR}} &= 2hcR_\infty \frac{r_{\mathrm{N}} Z^5 \alpha^3}{\pi n^3} \left\{ \mu_{\mathrm{r}}^3 \left[-\frac{8}{3} \ln k_0(n,l) - \frac{7}{3l(l+1)(2l+1)} \right] \right. \\
&\quad \left. + \pi Z \alpha \left[3 - \frac{l(l+1)}{n^2} \right] \frac{2}{(4l^2-1)(2l+3)} + \ldots \right\} \\
\alpha^2 D &= E_{\mathrm{D}} - 1; \quad r_{\mathrm{N}} = m_{\mathrm{e}}/m_{\mathrm{N}}; \quad \mu_r = 1/(1 + r_{\mathrm{N}})
\end{aligned}
$$

One-photon contribution to hydrogen-like levels

$$E_{\mathrm{SE}}^{(2)} = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}F(Z\alpha)\,m_{\mathrm{e}}c^2$$

$$\begin{aligned} F(Z\alpha) &= A_{41}\ln(Z\alpha)^{-2} + A_{40} + A_{50}\,(Z\alpha) + A_{62}\,(Z\alpha)^2\ln^2(Z\alpha)^{-2} \\ &\quad + A_{61}\,(Z\alpha)^2\ln(Z\alpha)^{-2} + G_{\mathrm{SE}}(Z\alpha)\,(Z\alpha)^2 \end{aligned}$$

$$F(Z\alpha) = A_{40} + A_{61}\,(Z\alpha)^2\ln(Z\alpha)^{-2} + G_{\mathrm{SE}}(Z\alpha)\,(Z\alpha)^2 \qquad l \geq 2$$

$$A_{40} = -\frac{4}{3}\ln k_0(n,l) - \frac{A_1^{(2)}}{\kappa(2l+1)} \qquad l \geq 2$$

$$G_{\mathrm{SE}}(Z\alpha) = A_{60} + \ldots$$

Two-photon contribution to hydrogen-like levels

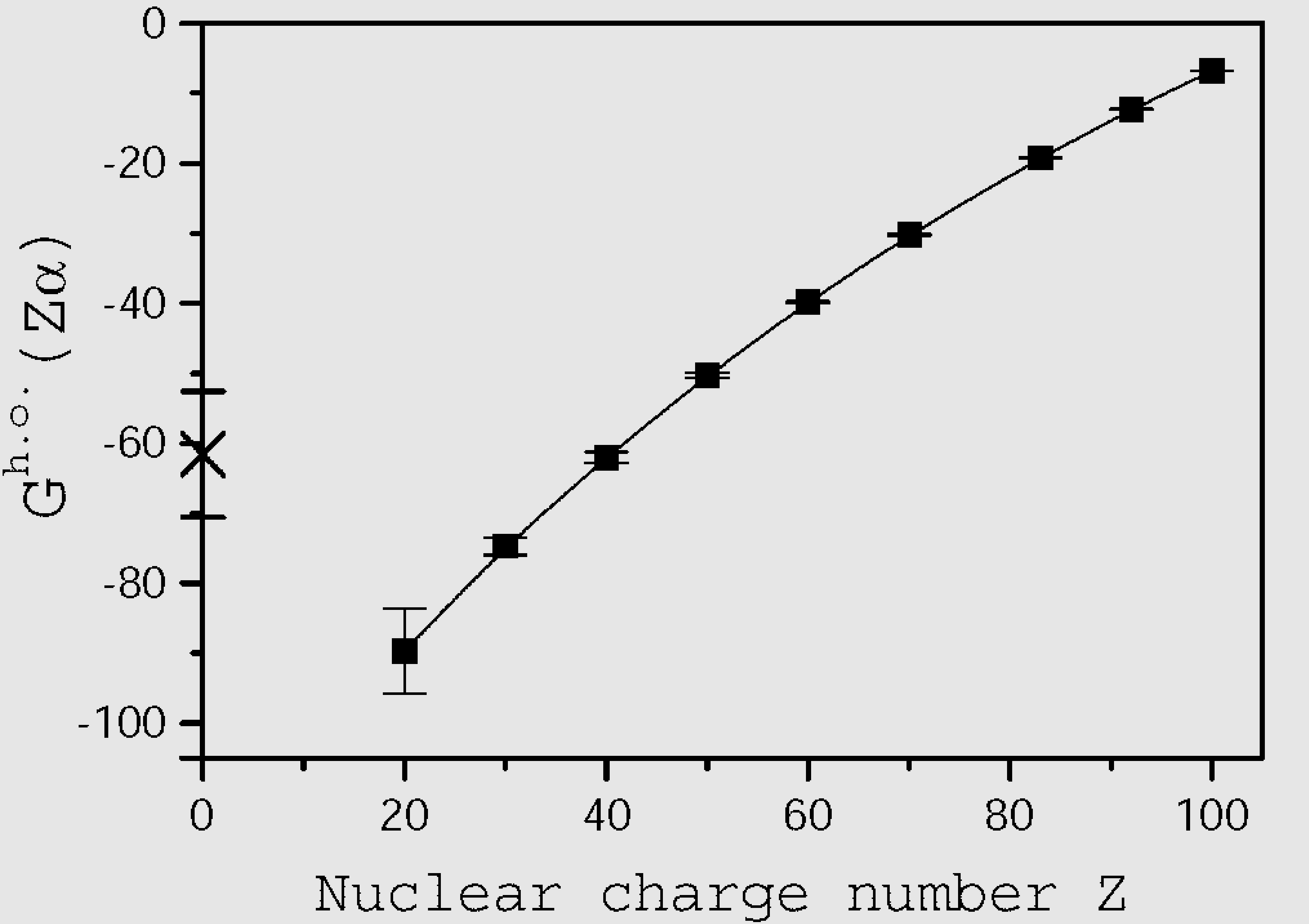
$$
\begin{aligned}
E^{(4)} &= \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^4}{n^3} m_{\rm e} c^2 F^{(4)}(Z\alpha) \\
F^{(4)}(Z\alpha) &= B_{40} + B_{50}\,(Z\alpha) + B_{63}\,(Z\alpha)^2 \ln^3 (Z\alpha)^{-2} \\
&\quad + B_{62}\,(Z\alpha)^2 \ln^2 (Z\alpha)^{-2} + B_{61}\,(Z\alpha)^2 \ln (Z\alpha)^{-2} + B_{60}\,(Z\alpha)^2 \\
&\quad + \cdots
\end{aligned}
$$

$$
F^{(4)}(Z\alpha) = B_{40} + B_{60}\,(Z\alpha)^2 + \cdots \qquad l \geq 2
$$

$$
B_{40} = -\frac{A_1^{(4)}}{\kappa(2l+1)} \qquad l \geq 2
$$

electron anomalous magnetic moment

$$
a_{\rm e}({\rm QED}) = A_1^{(2)}\left(\frac{\alpha}{\pi}\right) + A_1^{(4)}\left(\frac{\alpha}{\pi}\right)^2 + A_1^{(6)}\left(\frac{\alpha}{\pi}\right)^3 + A_1^{(8)}\left(\frac{\alpha}{\pi}\right)^4 + \cdots
$$



0
-20
-40
-60
-80
-100
0
20
40
60
80
100
$G^{h.o.}(Z\alpha)$
Nuclear charge number Z

Three- or more-photon contributions to hydrogen-like levels

$$E^{(6)} = \left(\frac{\alpha}{\pi}\right)^3 \frac{(Z\alpha)^4}{n^3} m_e c^2 \left[C_{40} + C_{60}(Z\alpha)^2 + \cdots\right] \qquad l \geq 2 \quad (?)$$

$$C_{40} = -\frac{A_1^{(6)}}{\kappa(2l+1)} \qquad l \geq 2$$

Total QED contribution to hydrogen-like levels

$$E_{\rm QED} = 2hcR_\infty \frac{Z^4\alpha^2}{n^3}\left\{ -\mu_r^2 \frac{a_e}{\kappa(2l+1)} + \mu_r^3 \frac{\alpha}{\pi}\left[-\frac{4}{3}\ln k_0(n,l) + \frac{32}{3}\frac{3n^2 - l(l+1)}{n^2} \right.\right.$$
$$\left.\left. \times \frac{(2l-2)!}{(2l+3)!}(Z\alpha)^2 \ln\left[\frac{1}{\mu_r(Z\alpha)^2}\right] + (Z\alpha)^2 G(Z\alpha)\right]\right\}$$

$$G(Z\alpha) = A_{60} + A_{81}(Z\alpha)^2 \ln (Z\alpha)^{-2} + A_{80}(Z\alpha)^2 + \ldots$$
$$+\frac{\alpha}{\pi} B_{60} + \ldots + \left(\frac{\alpha}{\pi}\right)^2 C_{60} + \ldots$$

Calculated values of A_{60}

- NRQED effective operators.
- Schrödinger Coulomb Green function on numerical grid.
- Sum over discrete-energy pseudo-state spectrum.
- B. Wundt poster on the calculation.

TABLE I. Calculated values of the constant A_{60}. The numbers in parentheses are standard uncertainties in the last figure.

n	l	$2j$	κ	A_{60}	$2j$	κ	A_{60}
13	11	21	11	$0.679\,575(5)\times 10^{-5}$	23	-12	$4.318\,998(5)\times 10^{-5}$
13	12	23	12	$0.469\,973(5)\times 10^{-5}$	25	-13	$2.729\,475(5)\times 10^{-5}$
14	12	23	12	$0.410\,825(5)\times 10^{-5}$	25	-13	$2.979\,937(5)\times 10^{-5}$
14	13	25	13	$0.296\,641(5)\times 10^{-5}$	27	-14	$1.945\,279(5)\times 10^{-5}$
15	13	25	13	$0.252\,108(5)\times 10^{-5}$	27	-14	$2.116\,050(5)\times 10^{-5}$
15	14	27	14	$0.189\,309(5)\times 10^{-5}$	29	-15	$1.420\,631(5)\times 10^{-5}$
16	14	27	14	$0.155\,786(5)\times 10^{-5}$	29	-15	$1.540\,181(5)\times 10^{-5}$
16	15	29	15	$0.121\,749(5)\times 10^{-5}$	31	-16	$1.059\,674(5)\times 10^{-5}$

TABLE II. Transition frequencies between the highest-j states with $n = 14$ and $n = 15$ in hydrogenlike helium and hydrogenlike neon.

Term	$^4He^+$ ν(THz)	$^{20}Ne^{9+}$ ν(THz)
E_{DM}	8.652 370 766 008(58)	216.335 625 5746(14)
E_{RR}	0.000 000 000 000	0.000 000 000 1
E_{QED}	−0.000 000 001 894	−0.000 001 184 1
Total	8.652 370 764 114(58)	216.335 624 3907(14)

TABLE III. Sources and estimated relative standard uncertainties in the theoretical value of the transition frequency between the highest-j states with $n = 14$ and $n = 15$ in hydrogenlike helium and hydrogenlike neon.

Source	He^+	Ne^{9+}
Rydberg constant	6.6×10^{-12}	6.6×10^{-12}
Fine-structure constant	7.0×10^{-16}	1.7×10^{-14}
Electron-nucleus mass ratio	5.8×10^{-14}	1.2×10^{-14}
a_e	5.1×10^{-20}	1.3×10^{-18}
Theory: E_{RR} higher order	6.2×10^{-17}	2.4×10^{-14}
Theory: $E_{QED}A_{81}$	1.7×10^{-18}	1.6×10^{-14}
Theory: $E_{QED}B_{60}$	8.6×10^{-18}	5.4×10^{-15}

Conclusion

- The current accuracy of the Rydberg constant is limited by uncertainties in the theory caused mainly by the proton charge radius.
- In Rydberg states of hydrogen-like atoms the overlap with the nucleus is extremely small.
- Higher-order binding effects in the QED corrections are suppressed in Rydberg states.
- Suitable combinations of n and Z provide Rydberg states with infrared or visible frequencies suitable for interrogation with a frequency comb.
- Measurement of the Rydberg constant in Rydberg states of hydrogen-like ions may be possible.