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

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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.

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)


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 - $R_\infty$ \[6.6 \times 10^{-12}\]
  - Proton rms charge radius - $R_p$ \[7.8 \times 10^{-3}\]
  - Deuteron rms charge radius - $R_d$ \[1.3 \times 10^{-3}\]

- 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 \[1.4 \times 10^{-14}\]
  - $R_p$ and $R_d$ electron scattering data
Rydberg constant from the LSA

Experiment:

\[ \nu_H(1S_{1/2} - 2S_{1/2}) = 2\,466\,061\,413\,187.074(34) \text{ kHz} \quad [1.4 \times 10^{-14}] \]

MPQ (2006)

Theory:

\[ \nu_H = \frac{3}{4} R_\infty c \left[ 1 - \frac{m_e}{m_p} + \frac{11}{48} \alpha^2 - \frac{28}{9} \frac{\alpha^3}{\pi} \ln \alpha^{-2} - \frac{14}{9} \left( \frac{\alpha R_p}{\lambda_C} \right)^2 + \ldots \right] \]

QED proton radius

Theory reviews:


Proton charge radius from 2006 least squares adjustment

\[ R_p \text{ e-p scatter (2003)} \]

\[ R_p \text{ LSA (2006)} \]
Transition frequencies in hydrogen and deuterium experiment - theory
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

\[ P(r) = \int_{|x| \leq r} \, \mathrm{d}x \, |\psi(x)|^2 \approx \frac{1}{(2n + 1)!} \left( \frac{2Zr}{na_0} \right)^{2n+1} \]
Transition frequencies in hydrogen-like ions
Electron probability to be inside radius $r$

hydrogen-like neon; $l = n - 1$

- $r = \text{nuclear radius}$
- $r = \text{Compton wavelength}$
Theory of Rydberg states for $l \geq 2$

\[ E_n = E_{DM} + E_{RR} + E_{QED} \]

\[ E_{DM} = 2\hbar c R_{\infty} \left[ \mu_r D - \frac{r_N \mu_r^3 \alpha^2}{2} D^2 + \frac{r_N^2 \mu_r^3 Z^4 \alpha^2}{2n^3 \kappa (2l + 1)} \right] \]

\[ E_{RR} = 2\hbar c R_{\infty} \frac{r_N Z^5 \alpha^3}{\pi n^3} \left\{ \mu_r^3 \left[ -\frac{8}{3} \ln k_0 (n, l) - \frac{7}{3l(l+1)(2l+1)} \right] \right. \]

\[ + \pi Z \alpha \left[ 3 - \frac{l(l+1)}{n^2} \right] \frac{2}{(4l^2 - 1)(2l + 3)} + \ldots \left\} \]

\[ \alpha^2 D = E_D - 1; \quad r_N = m_e/m_N; \quad \mu_r = 1/(1 + r_N) \]
One-photon contribution to hydrogen-like levels

\[ E^{(2)}_{SE} = \frac{\alpha (Z\alpha)^4}{\pi \frac{n^3}{\pi}} F(Z\alpha) m_e c^2 \]

\[ F(Z\alpha) = A_{41} \ln(Z\alpha)^{-2} + A_{40} + A_{50} (Z\alpha) + A_{62} (Z\alpha)^2 \ln^2(Z\alpha)^{-2} + A_{61} (Z\alpha)^2 \ln(Z\alpha)^{-2} + G_{SE}(Z\alpha) (Z\alpha)^2 \]

\[ F(Z\alpha) = A_{40} + A_{61} (Z\alpha)^2 \ln(Z\alpha)^{-2} + G_{SE}(Z\alpha) (Z\alpha)^2 \quad l \geq 2 \]

\[ A_{40} = -\frac{4}{3} \ln k_0(n, l) - \frac{A^{(2)}_1}{\kappa(2l + 1)} \quad l \geq 2 \]

\[ G_{SE}(Z\alpha) = A_{60} + \ldots \]
Two-photon contribution to hydrogen-like levels

\[ E^{(4)} = \left( \frac{\alpha}{\pi} \right)^2 \frac{(Z\alpha)^4}{n^3} m_e c^2 F^{(4)}(Z\alpha) \]

\[ F^{(4)}(Z\alpha) = B_{40} + B_{50} (Z\alpha) + B_{63} (Z\alpha)^2 \ln^3(Z\alpha)^{-2} + B_{62} (Z\alpha)^2 \ln^2(Z\alpha)^{-2} + B_{61} (Z\alpha)^2 \ln(Z\alpha)^{-2} + B_{60} (Z\alpha)^2 + \cdots \]

\[ F^{(4)}(Z\alpha) = B_{40} + B_{60} (Z\alpha)^2 + \cdots \quad l \geq 2 \]

\[ B_{40} = -\frac{A_1^{(4)}}{\kappa(2l + 1)} \quad l \geq 2 \]

electron anomalous magnetic moment

\[ a_e(QED) = A_1^{(2)} \left( \frac{\alpha}{\pi} \right) + A_1^{(4)} \left( \frac{\alpha}{\pi} \right)^2 + A_1^{(6)} \left( \frac{\alpha}{\pi} \right)^3 + A_1^{(8)} \left( \frac{\alpha}{\pi} \right)^4 + \cdots \]
Three- or more-photon contributions to hydrogen-like levels

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

\[
C_{40} = -\frac{A_1^{(6)}}{\kappa(2l + 1)} \quad l \geq 2
\]

Total QED contribution to hydrogen-like levels

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

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

<table>
<thead>
<tr>
<th>$n$</th>
<th>$l$</th>
<th>$2j$</th>
<th>$\kappa$</th>
<th>$A_{60}$</th>
<th>$2j$</th>
<th>$\kappa$</th>
<th>$A_{60}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>11</td>
<td>21</td>
<td>11</td>
<td>0.679 575(5) × 10$^{-5}$</td>
<td>23</td>
<td>−12</td>
<td>4.318 998(5) × 10$^{-5}$</td>
</tr>
<tr>
<td>13</td>
<td>12</td>
<td>23</td>
<td>12</td>
<td>0.469 973(5) × 10$^{-5}$</td>
<td>25</td>
<td>−13</td>
<td>2.729 475(5) × 10$^{-5}$</td>
</tr>
<tr>
<td>14</td>
<td>12</td>
<td>23</td>
<td>12</td>
<td>0.410 825(5) × 10$^{-5}$</td>
<td>25</td>
<td>−13</td>
<td>2.979 937(5) × 10$^{-5}$</td>
</tr>
<tr>
<td>14</td>
<td>13</td>
<td>25</td>
<td>13</td>
<td>0.296 641(5) × 10$^{-5}$</td>
<td>27</td>
<td>−14</td>
<td>1.945 279(5) × 10$^{-5}$</td>
</tr>
<tr>
<td>15</td>
<td>13</td>
<td>25</td>
<td>13</td>
<td>0.252 108(5) × 10$^{-5}$</td>
<td>27</td>
<td>−14</td>
<td>2.116 050(5) × 10$^{-5}$</td>
</tr>
<tr>
<td>15</td>
<td>14</td>
<td>27</td>
<td>14</td>
<td>0.189 309(5) × 10$^{-5}$</td>
<td>29</td>
<td>−15</td>
<td>1.420 631(5) × 10$^{-5}$</td>
</tr>
<tr>
<td>16</td>
<td>14</td>
<td>27</td>
<td>14</td>
<td>0.155 786(5) × 10$^{-5}$</td>
<td>29</td>
<td>−15</td>
<td>1.540 181(5) × 10$^{-5}$</td>
</tr>
<tr>
<td>16</td>
<td>15</td>
<td>29</td>
<td>15</td>
<td>0.121 749(5) × 10$^{-5}$</td>
<td>31</td>
<td>−16</td>
<td>1.059 674(5) × 10$^{-5}$</td>
</tr>
</tbody>
</table>
TABLE II. Transition frequencies between the highest-$j$ states with $n = 14$ and $n = 15$ in hydrogenlike helium and hydrogen-like neon.

<table>
<thead>
<tr>
<th>Term</th>
<th>$^4\text{He}^+$ $\nu$(THz)</th>
<th>$^{20}\text{Ne}^{9+}$ $\nu$(THz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{\text{DM}}$</td>
<td>8.652 370 766 008(58)</td>
<td>216.335 625 5746(14)</td>
</tr>
<tr>
<td>$E_{\text{RR}}$</td>
<td>0.000 000 000 000</td>
<td>0.000 000 000 10</td>
</tr>
<tr>
<td>$E_{\text{QED}}$</td>
<td>-0.000 000 001 894</td>
<td>-0.000 001 184 1</td>
</tr>
<tr>
<td>Total</td>
<td>8.652 370 764 114(58)</td>
<td>216.335 624 3907(14)</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Source</th>
<th>$\text{He}^+$</th>
<th>$\text{Ne}^{9+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rydberg constant</td>
<td>$6.6 \times 10^{-12}$</td>
<td>$6.6 \times 10^{-12}$</td>
</tr>
<tr>
<td>Fine-structure constant</td>
<td>$7.0 \times 10^{-16}$</td>
<td>$1.7 \times 10^{-14}$</td>
</tr>
<tr>
<td>Electron-nucleus mass ratio</td>
<td>$5.8 \times 10^{-14}$</td>
<td>$1.2 \times 10^{-14}$</td>
</tr>
<tr>
<td>$a_e$</td>
<td>$5.1 \times 10^{-20}$</td>
<td>$1.3 \times 10^{-18}$</td>
</tr>
<tr>
<td>Theory: $E_{\text{RR}}$ higher order</td>
<td>$6.2 \times 10^{-17}$</td>
<td>$2.4 \times 10^{-14}$</td>
</tr>
<tr>
<td>Theory: $E_{\text{QED}}A_{81}$</td>
<td>$1.7 \times 10^{-18}$</td>
<td>$1.6 \times 10^{-14}$</td>
</tr>
<tr>
<td>Theory: $E_{\text{QED}}B_{60}$</td>
<td>$8.6 \times 10^{-18}$</td>
<td>$5.4 \times 10^{-15}$</td>
</tr>
</tbody>
</table>
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.